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Title:	Caveat Emptor! Uncertainties are Uncertain. Changes in ENDF/B-VIII.0 Uncertainties to Reproduce Issues in Underlying Measurements and Theory.
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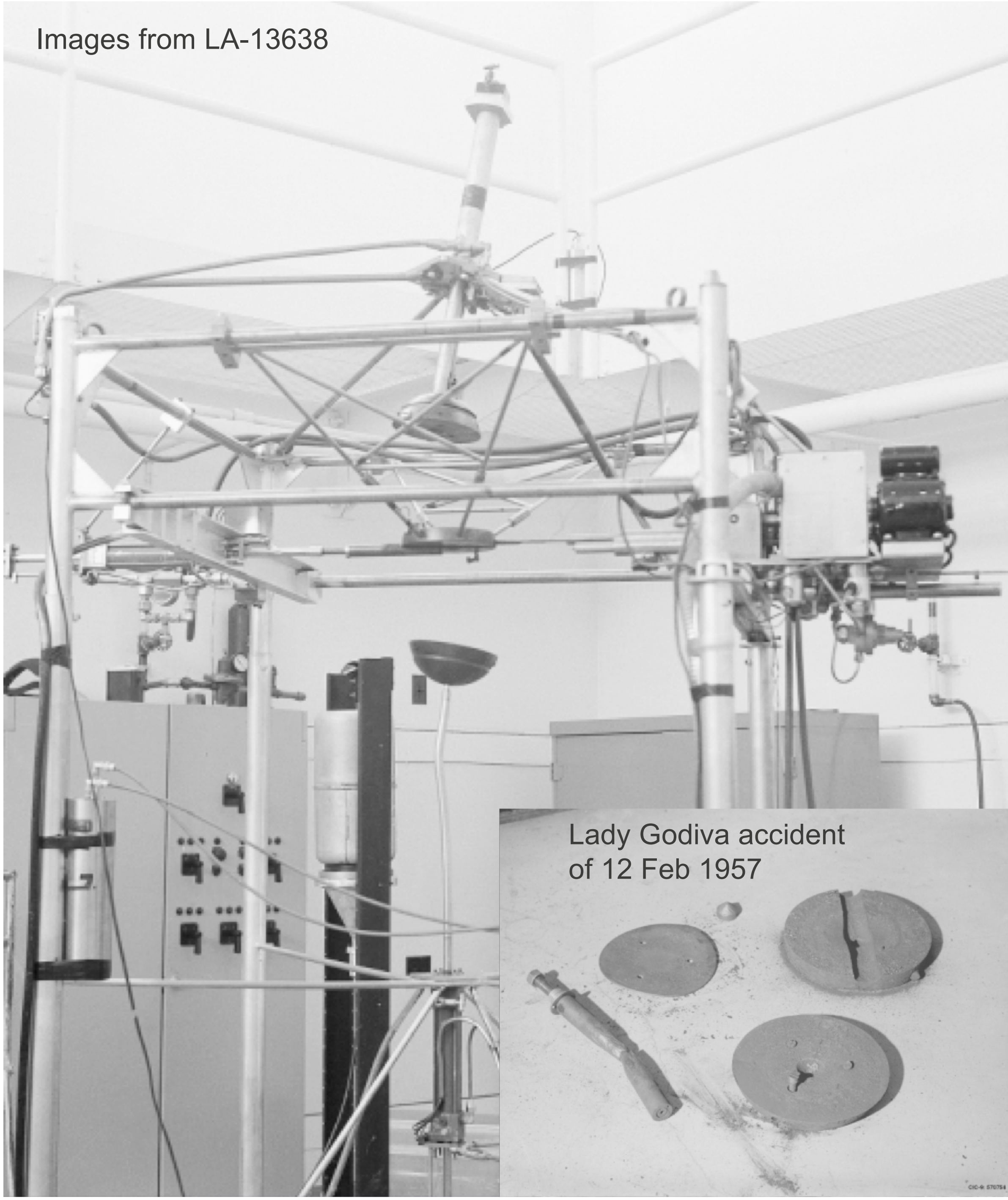
Caveat Emptor! Uncertainties are Uncertain

Changes in ENDF/B-VIII.0 Uncertainties to Reproduce Issues in Underlying Measurements and Theory

Morgan C. White

9th Trilab Nuclear Data Workshop (NDW9)
26 February – 2 March, 2018

Images from LA-13638



Lady Godiva accident of 12 Feb 1957

Los Alamos
NATIONAL LABORATORY
EST. 1943

Delivering science and technology
to protect our nation
and promote world stability

NNSA
National Nuclear Security Administration

True, or Not True
Past Performance is no Guarantee of Future Results*

- **The central question we have asked through the ages is essentially, “will it work?” Will this process produce the result I want?**
  - This question is very limited in scope, with results that can be checked by executing the process; more so, results that are ‘good enough’ are often acceptable
  - We are very good at predicting the likely future. Our daily life proves this so.
  - So why do we fail so often to predict a surprise…

- **Little attention is paid to the follow on question, “how certain are you it will work?” Will this process fail to produce the necessary result?**
  - This question lays bare the world…
  - One needs a healthy dose of reality to ensure that the answer, ‘well, the meteorite is going to hit and nothing is going to work anyway’ doesn’t rule the day
  - But we typically don’t care about the average *good enough* answer, we are worried about the *corner cases* where an unlikely, *but possible*, set of circumstances bring about an unexpected failure

* Consumer warning required in investment advertising per SEC Rule 156

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A strong science program is our only mitigation against surprise.

Conservative versus Realistic versus I don’t know Differences in Philosophy Matter

- **Many groups want systematic error estimates to be conservative**
  - By this, they generally mean they really want a bound on what might happen
    - Might this configuration go critical, or fail to go critical
    - Could this transient cause enough heating/dose to melt/damage these parts
  - These are examples of what I call *corner cases*
  - To provide such estimates, one *must* address *unknown unknowns*
- **Those who want “realistic” errors often look at how well we are able to “predict” their systems and demand we reduce our error estimates**
  - There is a general misunderstanding that our process to calibrate our mean values somehow reduces the uncertainties on underlying data
  - Error quantification is a multi-level process where having a benchmark that resembles the system of interest can help constrain near neighbor predictions
    - If we already know the answer, we often confuse *calibrations* with *predictions*
- **And then there is the moral and ethical quandary of trying to quantify what we do not know**
  - How does one put a number on an *unknown unknown*
  - But computers do what you tell them and *I don’t know == 0*

Known knowns
- mathematically rigorous definitions

Known unknowns
- scientifically measurable perception of reality

Unknown unknowns
- nature intruding on good ideas

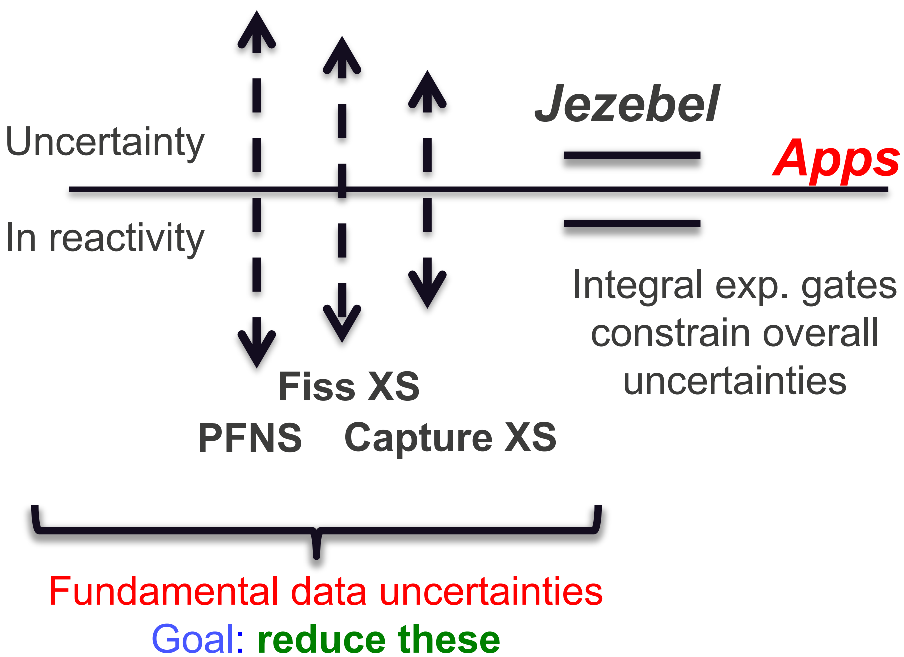
Unknown knowns
- scientific, or not, wonderfully astute guess sWAGs

Uncertainties in our fundamental data would have even larger impact without integral constraints.

- Overall nuclear reactivity is constrained by exceptionally precise criticality experiments – especially Jezebel (bare Pu), Godiva (bare HEU), and SNM + reflectors (e.g. U, Be, Fe, Poly, …)
- But there are compensating errors in the XS components that drive reactivity that are much larger than this constraint.
- **One can get criticality right for the wrong reasons, and then get other things wrong, e.g. diagnostics, outputs and performance!**
- -> *example: a recent trial (softer) prompt fission neutron spectrum (PFNS) for Pu239 reduced the (n,2n) reaction rate in Jezebel by ~10% [Kahler LA-UR-14-28703] with implications on metrics like deltaP*

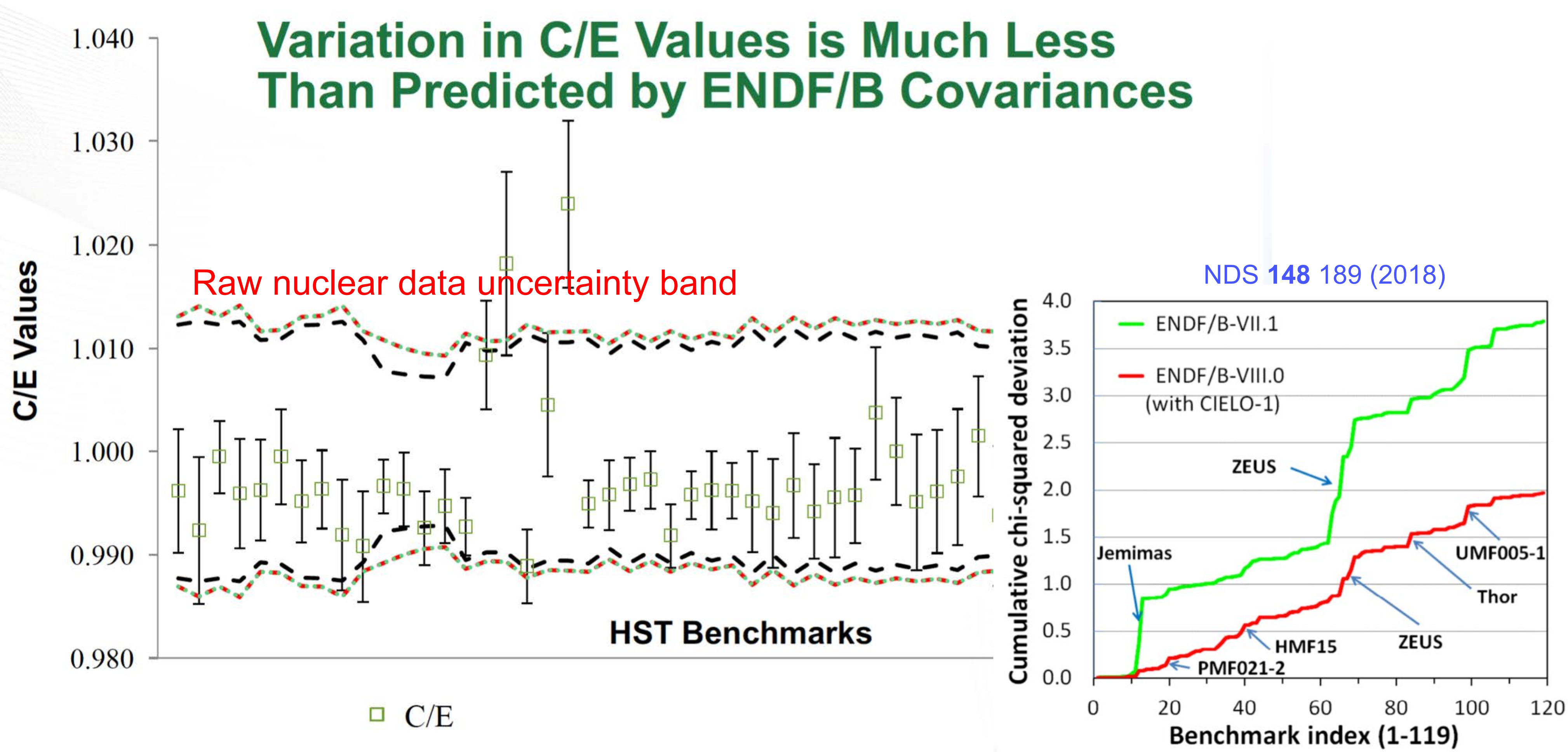
We rarely understand the impact of errors in isolation.

They interact, often in unexpected ways.



Calibration is the art of selecting compensating errors that match our 'gates' better than deserved…

M. Williams, B.J. Marshall, CSEWG 2017.



Left 'unknobbed' our data would have a spread of C/E values surrounding the bands. ND 'evaluations' recognize the importance of these means and selectively tunes suites of data to meet a level of performance for applications.

The 2018 International Standards and ENDF/B-VIII.0 Have Dramatically Increased (often 2x) Many Variances

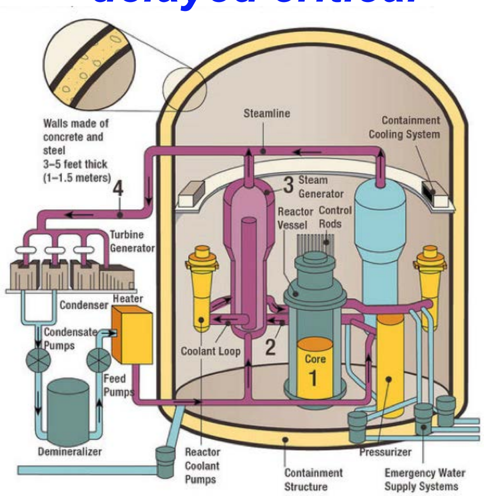
- **Our community and our users** ***should question this assertion***
  - On what basis where the old errors given?
  - What were we missing that we understated the issues within these data?
  - What new, or newly understood, information forms the basis for the current estimate?
  - …

- **The remainder of this talk provides an overview of**
  - many of the issues we have seen,
  - what we have learned,
  - and how we are trying to use this information to update our error quantifications.

One dollar ($) is the difference between steady state and a bad day.

The neutron reactivity scale

Steady energy production at *delayed critical*



"Lady Godiva" before and after prompt excursion of ~10 cents

Runaway energy production above *prompt critical*

$$\frac{1}{v(E)}\frac{\partial\psi(\mathbf{r},E,\hat{\boldsymbol{\Omega}},t)}{\partial t}+\hat{\boldsymbol{\Omega}}\cdot\nabla\psi(\mathbf{r},E,\hat{\boldsymbol{\Omega}},t)+\Sigma_t(\mathbf{r},E,t)\,\psi(\mathbf{r},E,\hat{\boldsymbol{\Omega}},t)=$$
$$\frac{\chi_p(E)}{4\pi}\int_0^\infty dE'\nu_p(E')\,\Sigma_f(\mathbf{r},E',t)\,\phi(\mathbf{r},E',t)+\cancel{\sum_{i=1}^{N}\frac{\chi_{di}(E)}{4\pi}\lambda_i C_i(\mathbf{r},t)}+$$
$$\int_{4\pi}d\Omega'\int_0^\infty dE'\,\Sigma_s(\mathbf{r},E'\to E,\hat{\boldsymbol{\Omega}}'\to\hat{\boldsymbol{\Omega}},t)\psi(\mathbf{r},E',\hat{\boldsymbol{\Omega}}',t)+s(\mathbf{r},E,\hat{\boldsymbol{\Omega}},t)$$

Prompt critical is steady state neutron production without delayed neutrons

Boltzmann equation

The Data Dilemma
Beware of Atoms, They Make Up Everything

- **If you have no data, you get to make it up**
- **If you have one data set, it must be correct**
- **If you have two data sets, they are both wrong**
  - And everyone is just going to pick their favorite
  - Or worse, take the average of the two
- **When you have many data sets, you get to make it up again**

It is not enough to make the most accurate measurement.

It will always be viewed within its historic context and we must understand the previous systematic errors.

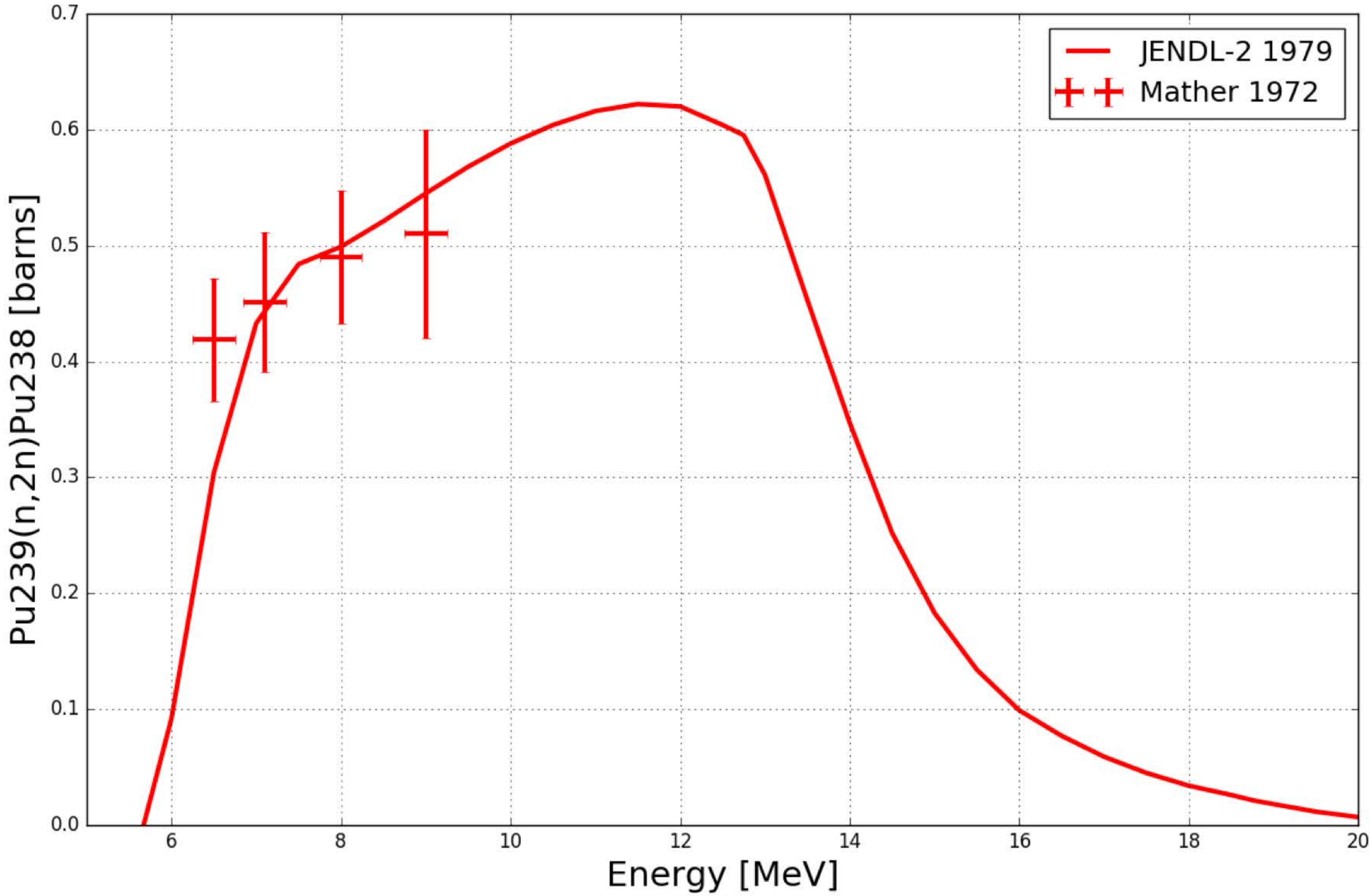
Pu239(n,2n)Pu238

Small, < 20 cents compared to $$, impact on reactivity

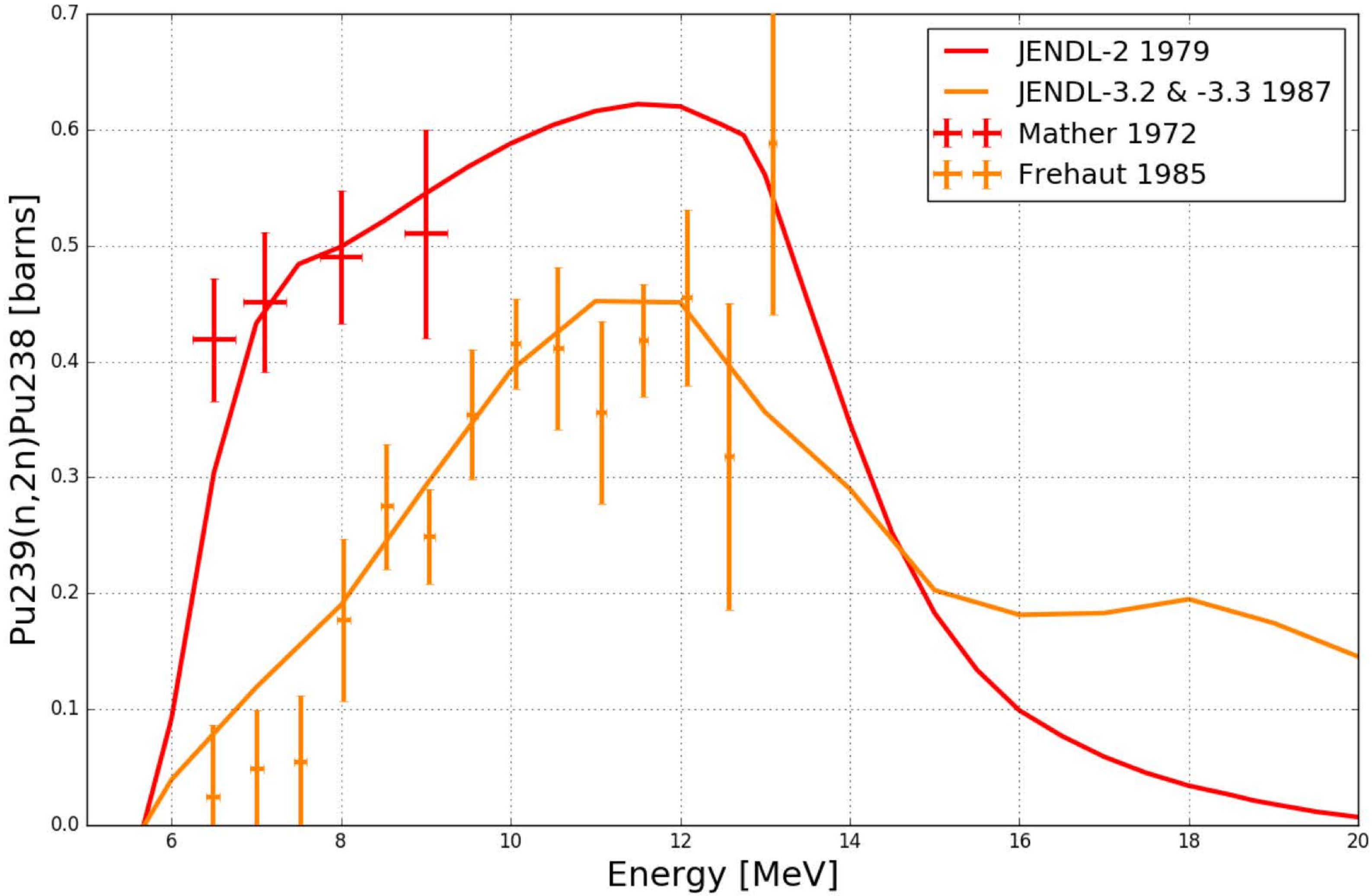
Impacts Δ Plutonium Radiochemistry

But a great example of the data dilemma…

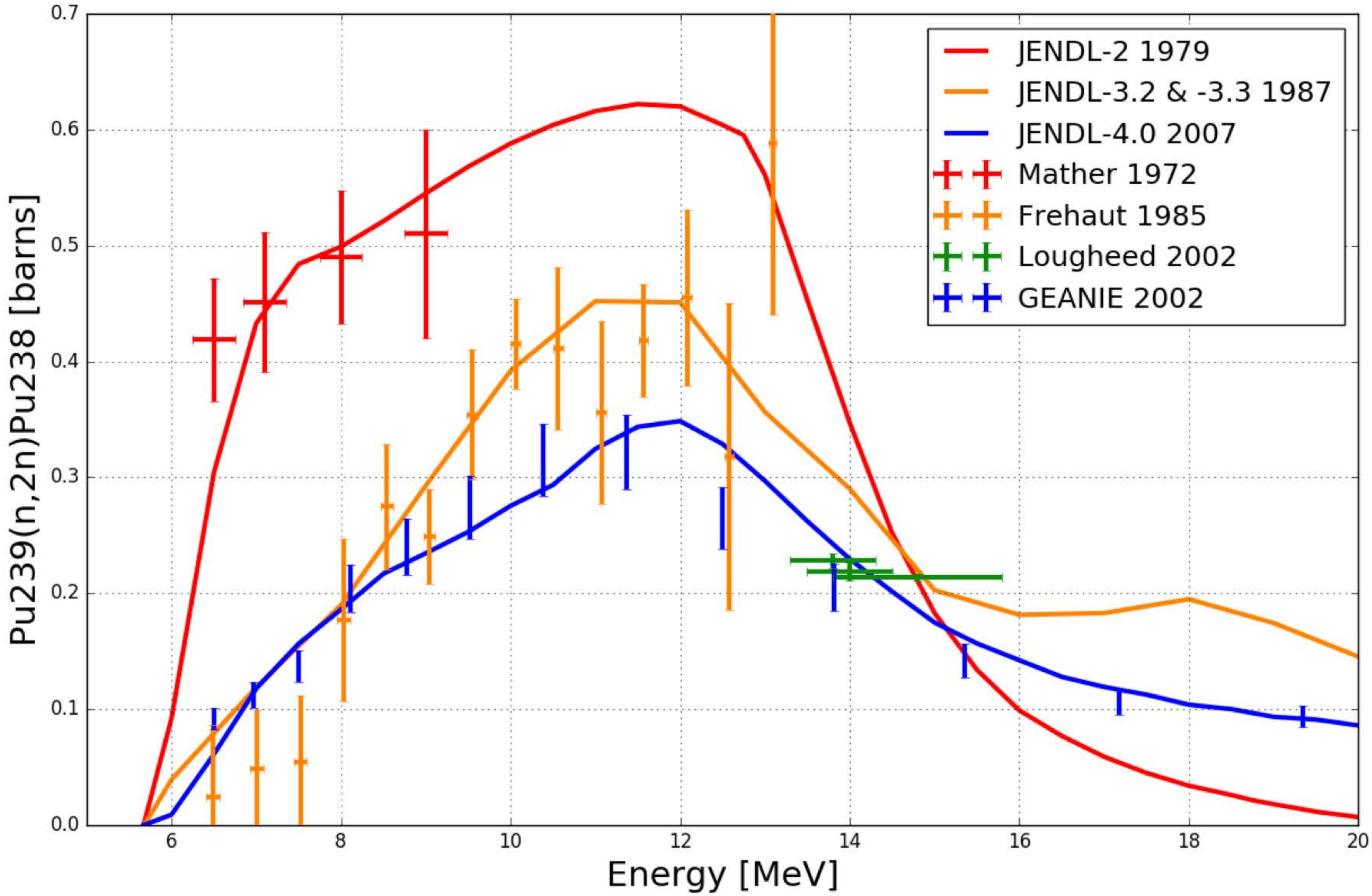
If you have one data set, it must be correct.



If you have two data sets, they are both wrong. And everyone is just going to pick their favorite.



(And everyone is just going to pick their favorite.) Latest and greatest! It must be better.



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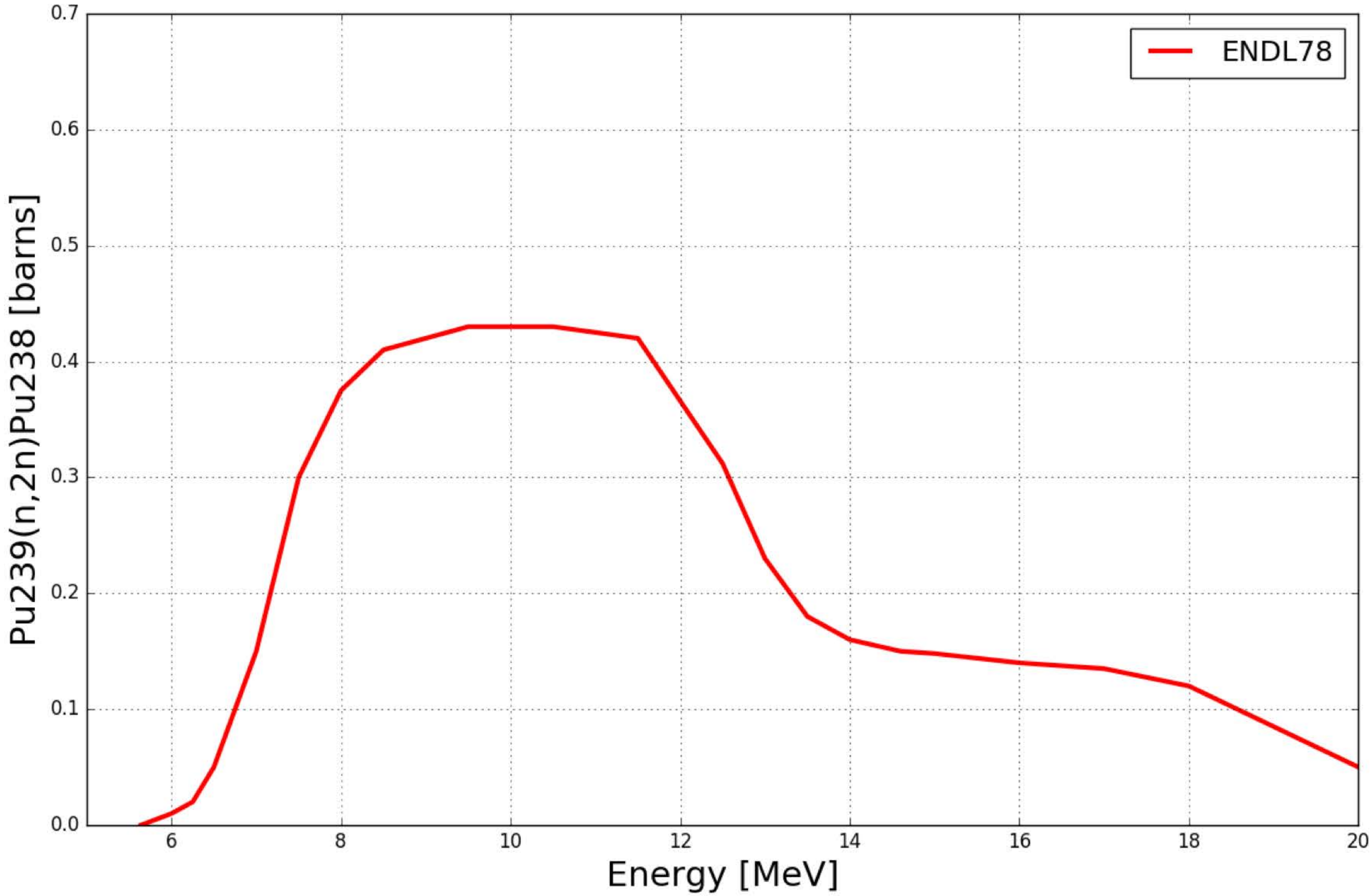

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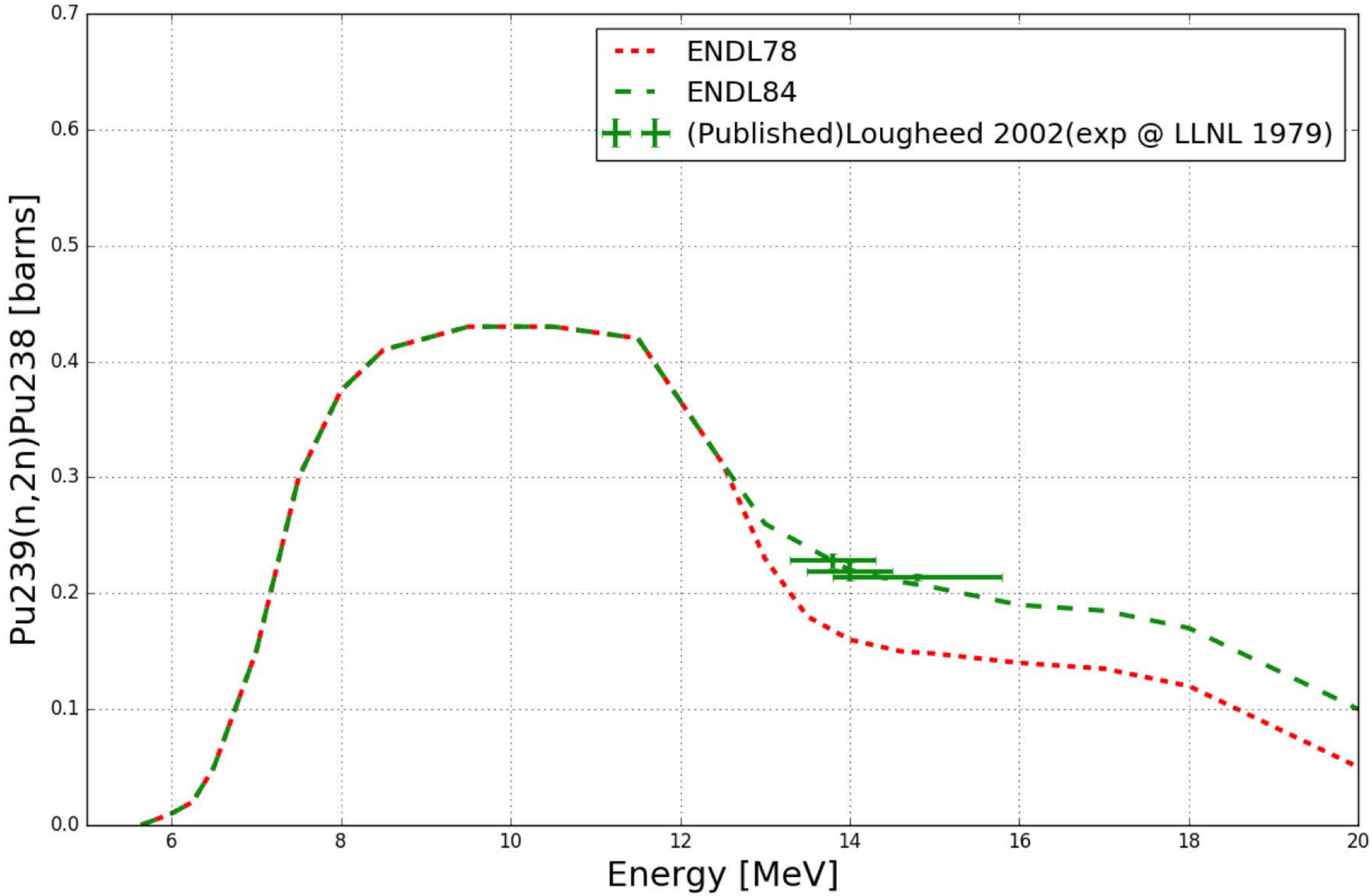

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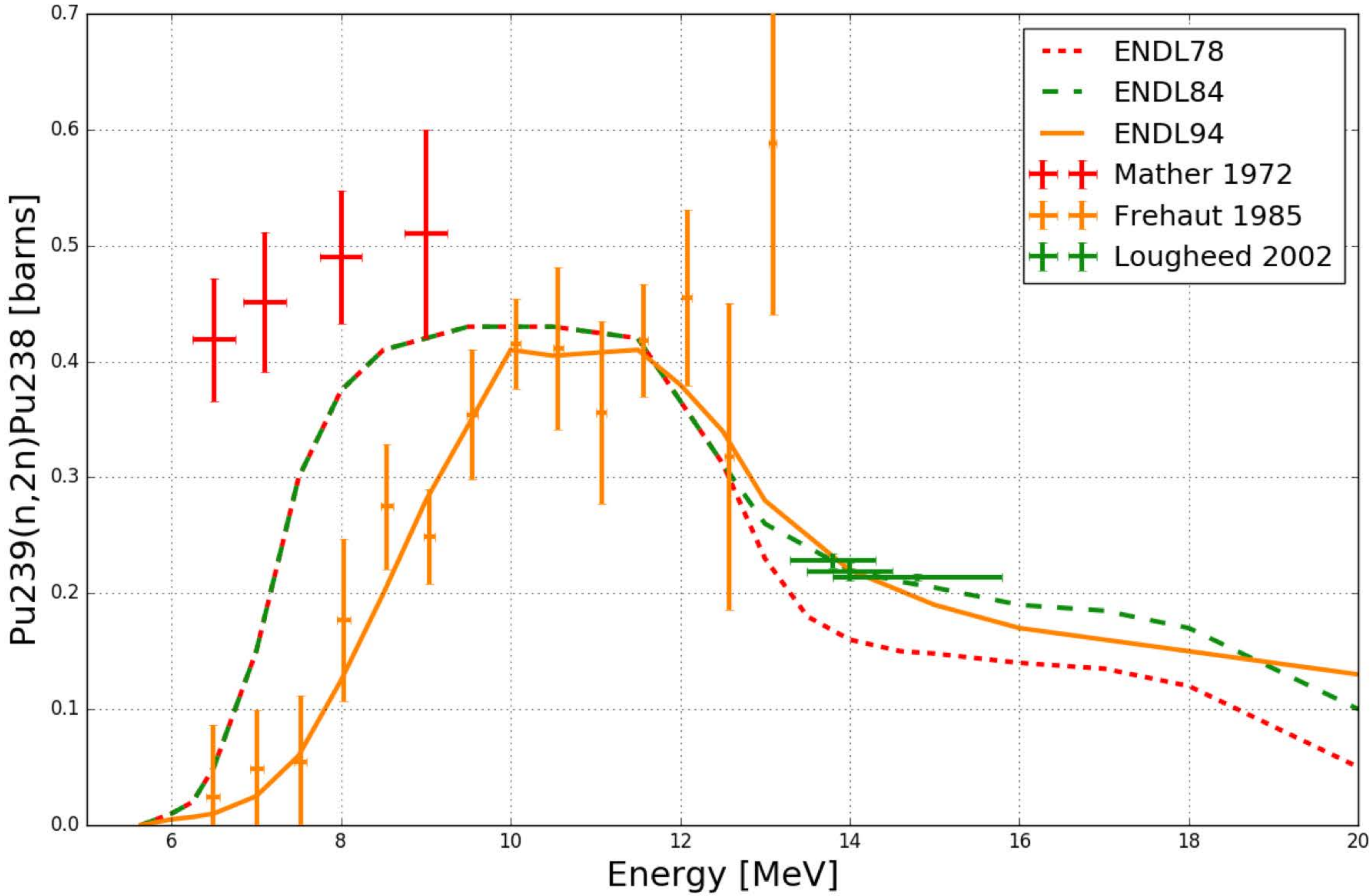
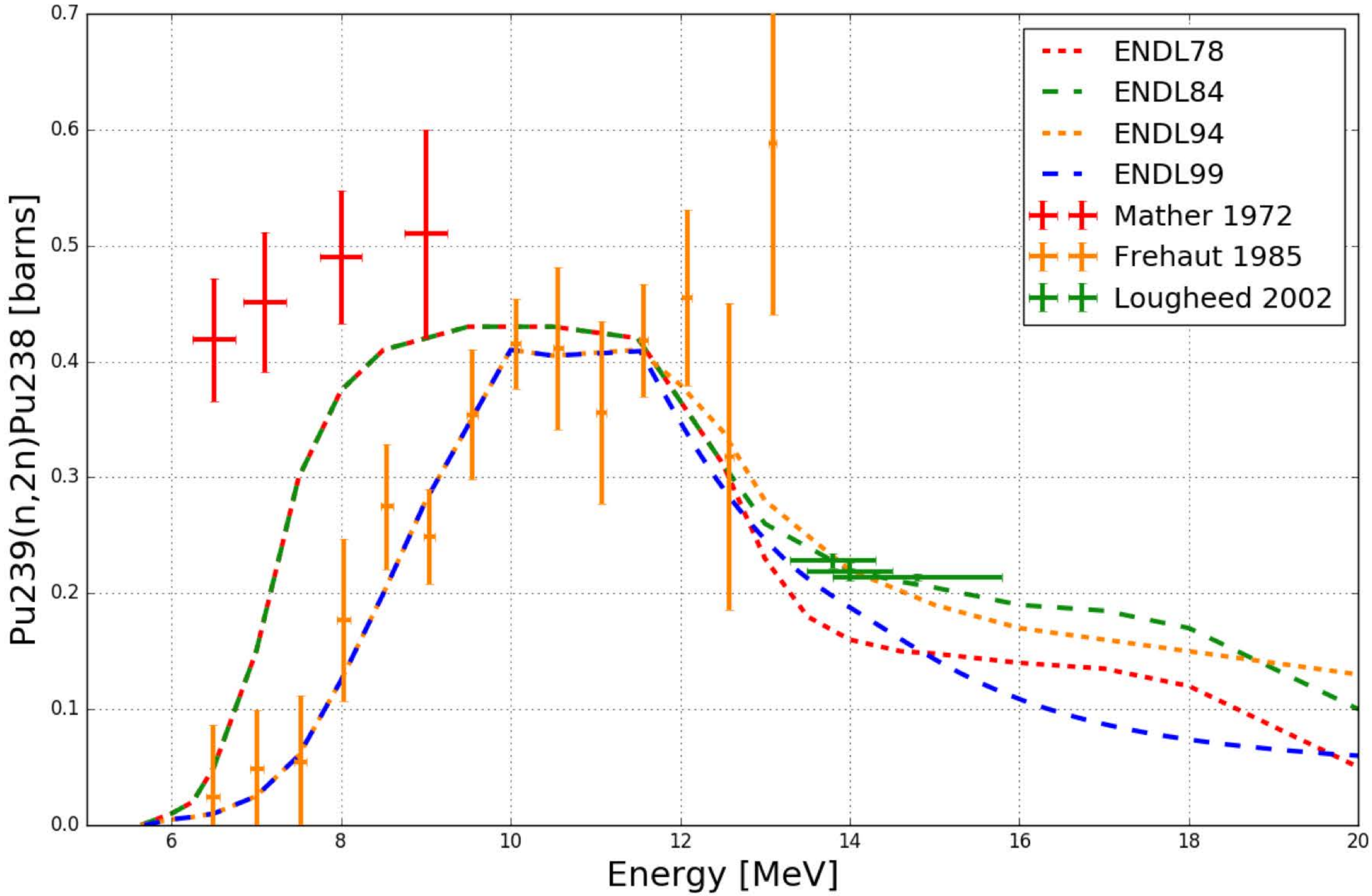
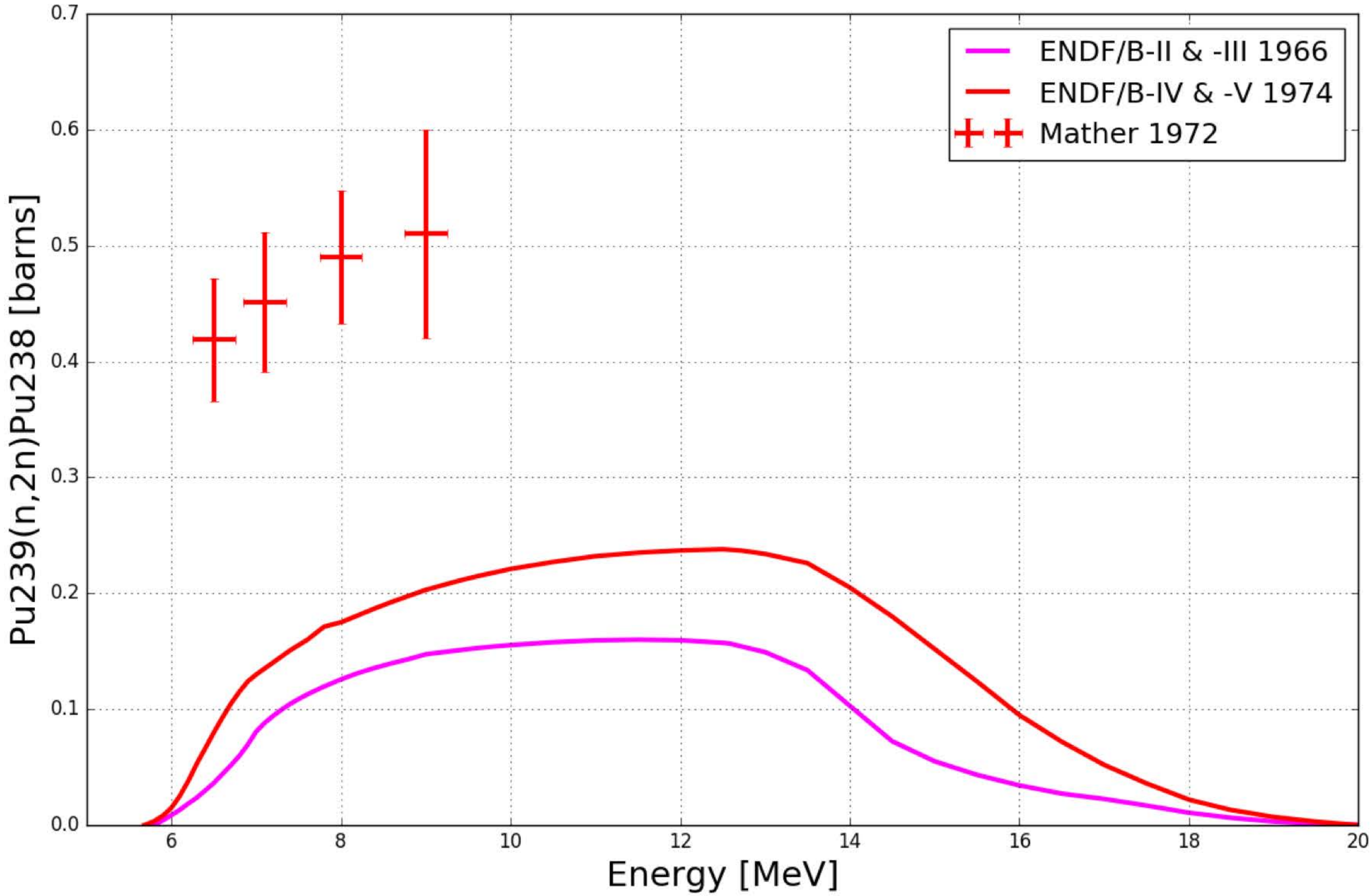


And some days you just have to wonder…

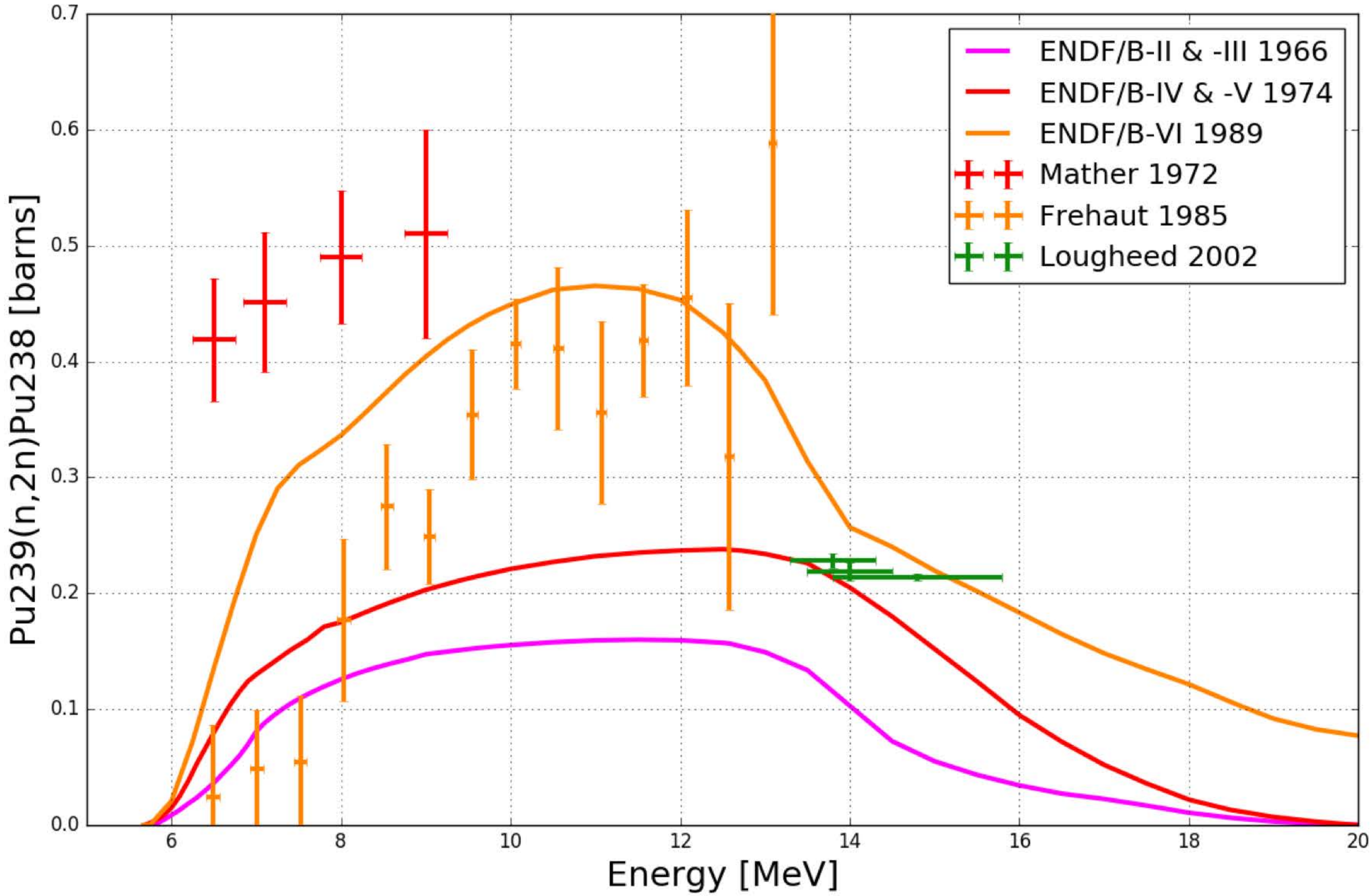
(The evaluation at 14 MeV moves 15% away from the data.)



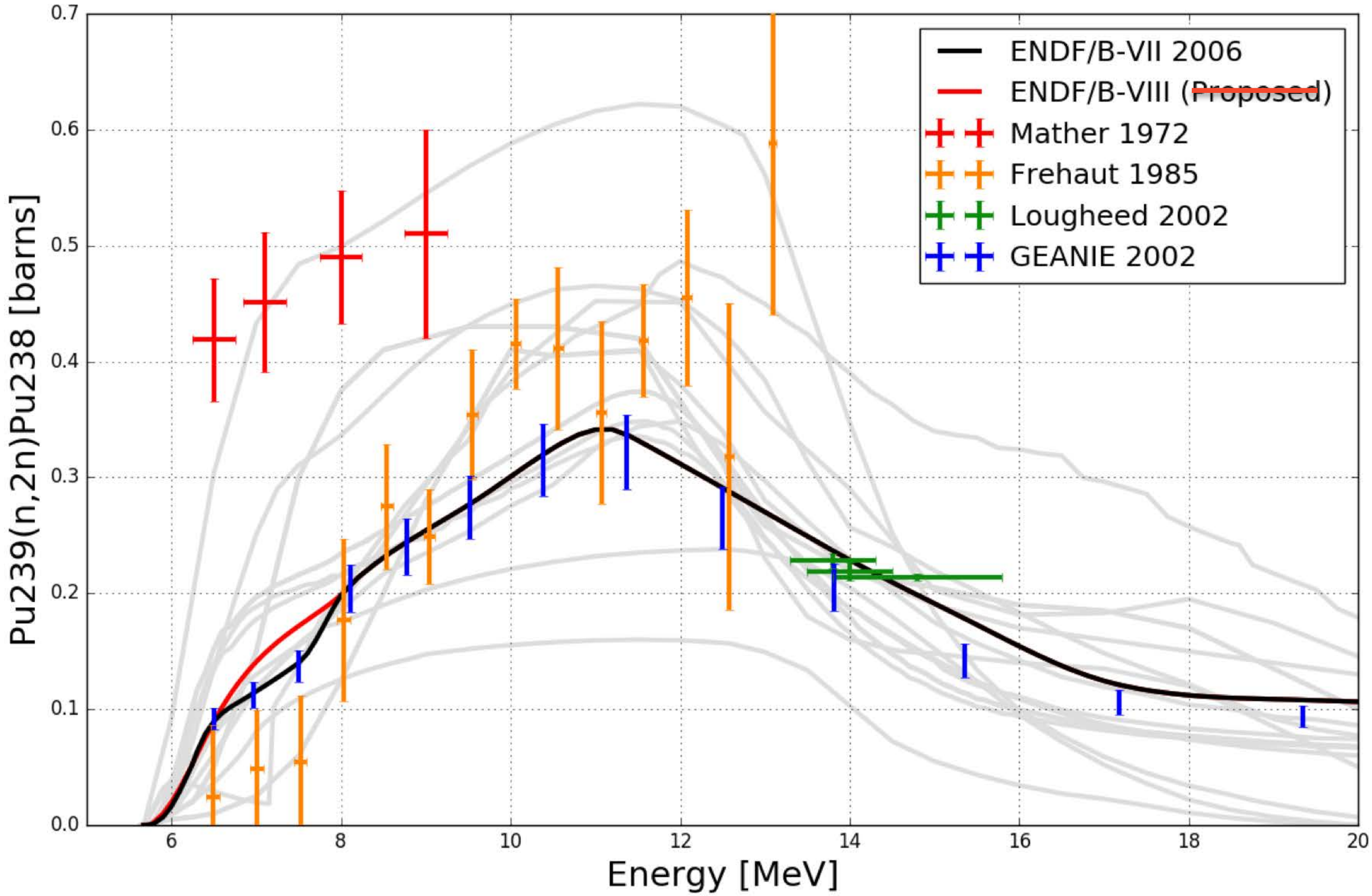
Maybe you should just ignore the data.
They are obviously wrong, right?



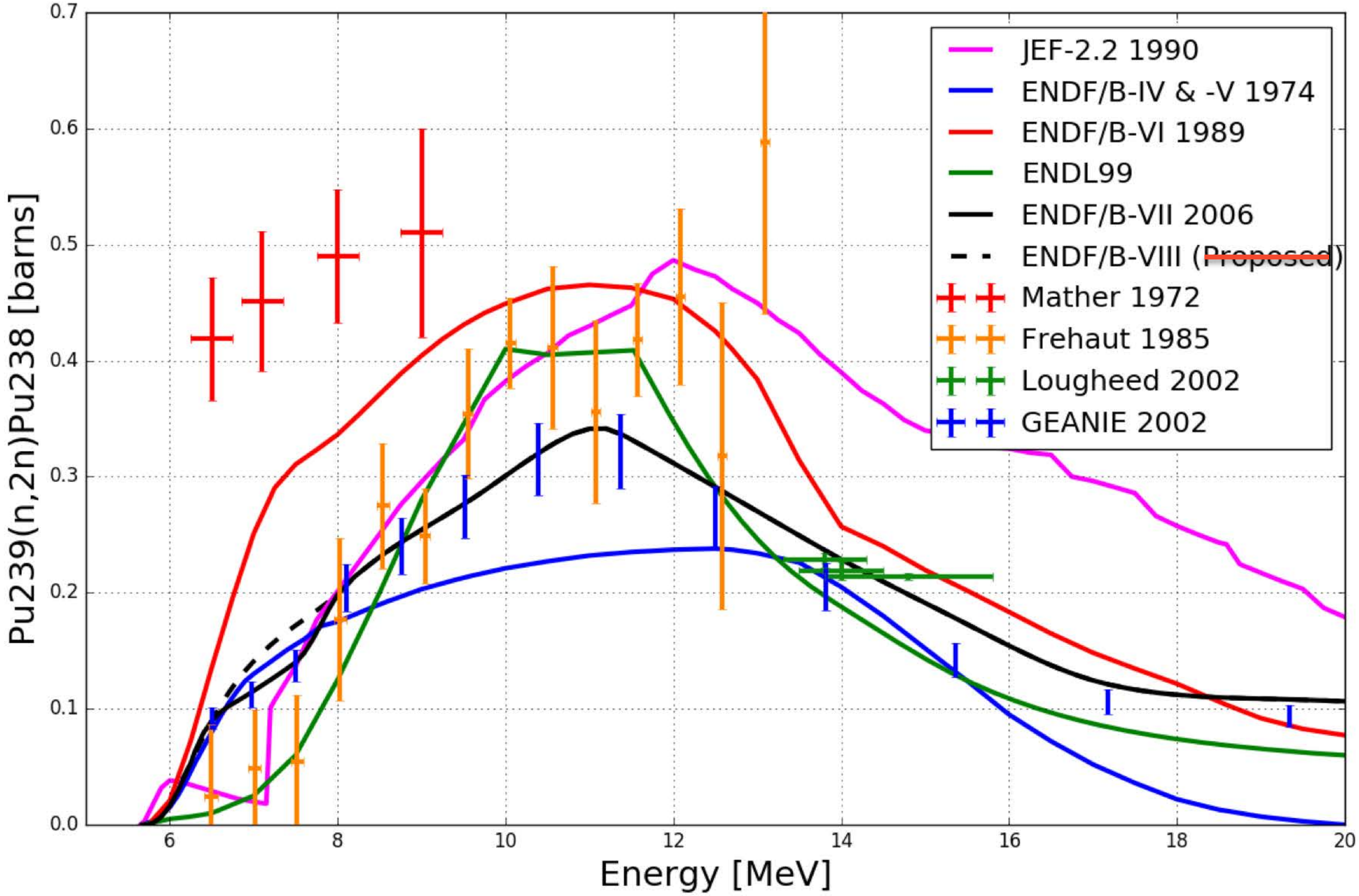
Or is it better to split the difference. And declare the error to be smaller than either!



The ENDF/B-VIII.0 Pu239(n,2n)Pu238 Cross Section Eliminates an Unphysical Inflection Near Threshold



History of the Pu239(n,2n)Pu238 Cross Section at LANL, LLNL and AWE

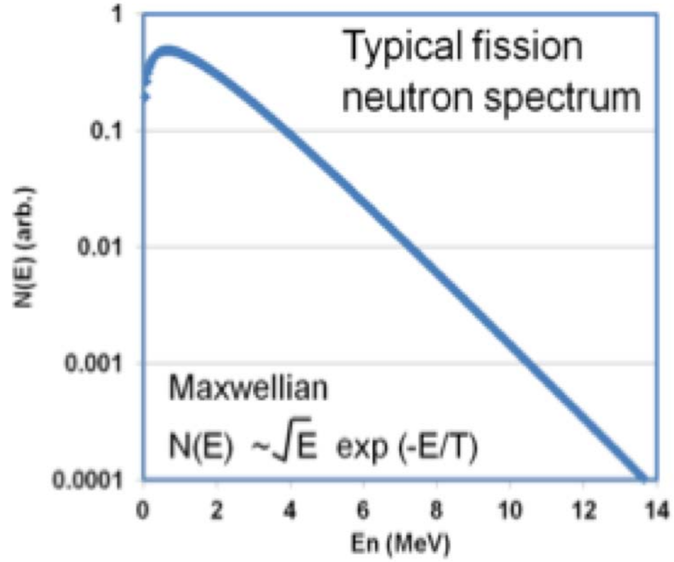


Pu239 Prompt Fission Neutron Spectra (PFNS)
The fission source term: $\Psi\ \nu\ \sigma\ \chi$

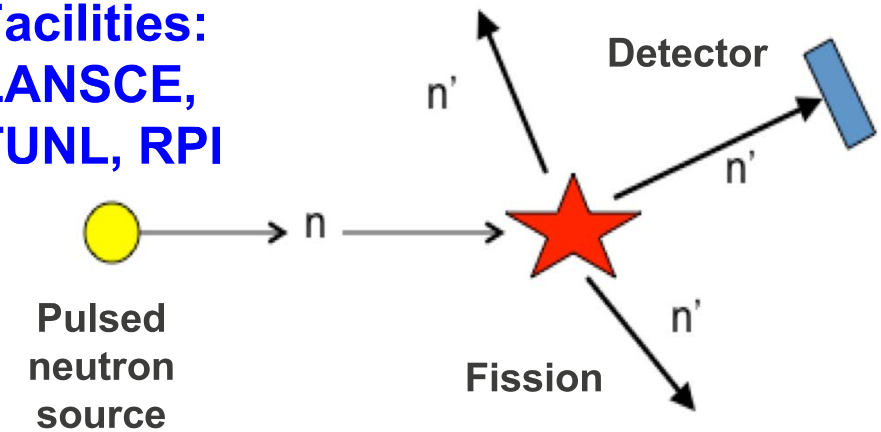
Chi

Measuring the prompt fission neutron spectra (PFNS) is straightforward in principle, but *there are challenges*…

- Measure incident and emission energies through a double-time-of-flight detector
- Need fast timing signals for the neutron production, fission, and emission neutron times measured over well-known path lengths



Facilities: LANSCE, TUNL, RPI



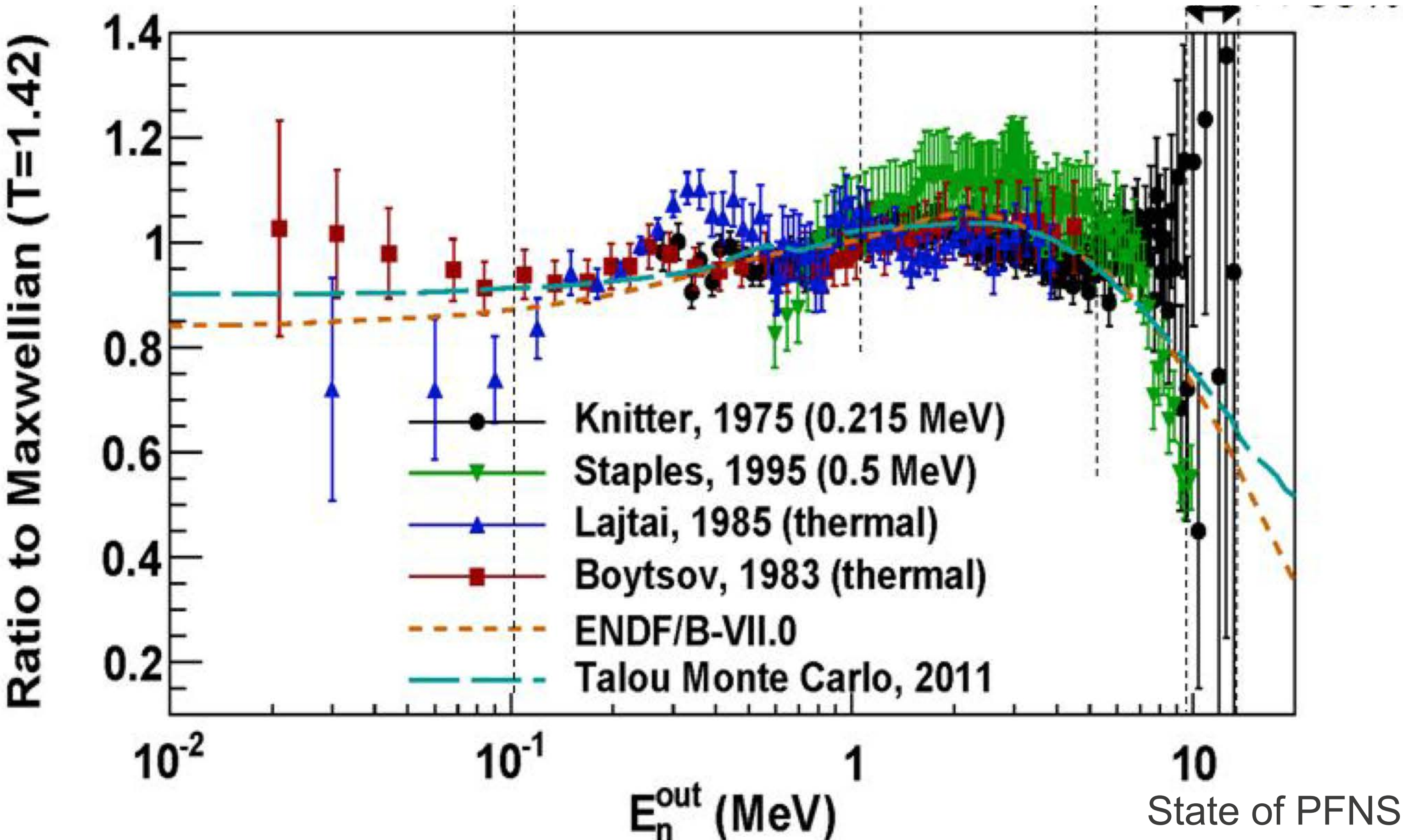
The challenges are in:

- neutron scattering
  - fouls up path length
  - neutrons scatter to lower energy changing there detection efficiency
- backgrounds
- good timing (ns)
- detector response
- neutron-gamma separation
- few neutrons at high energies
- *fission fragment anisotropic emission*

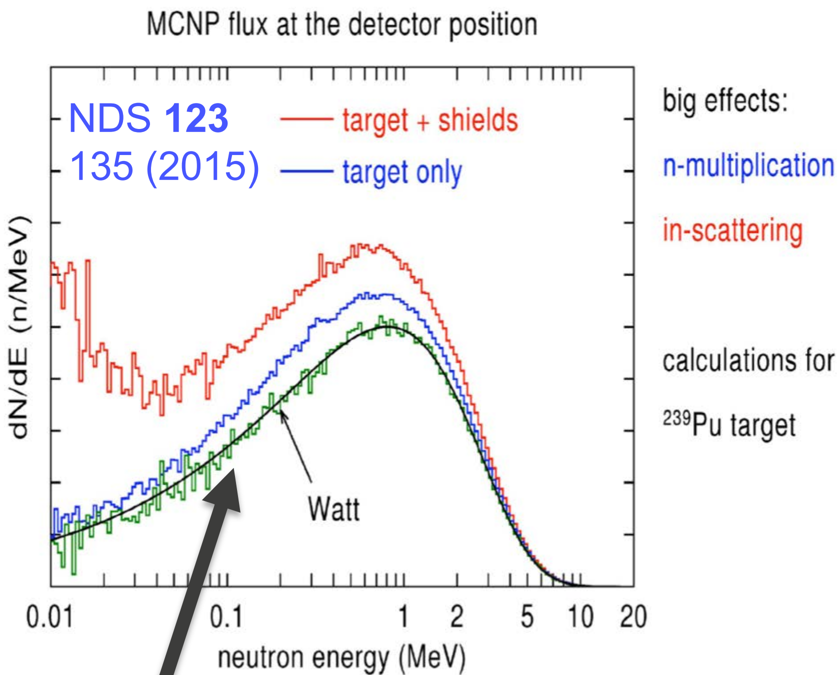
Two key advances enabled new error estimates for PFNS

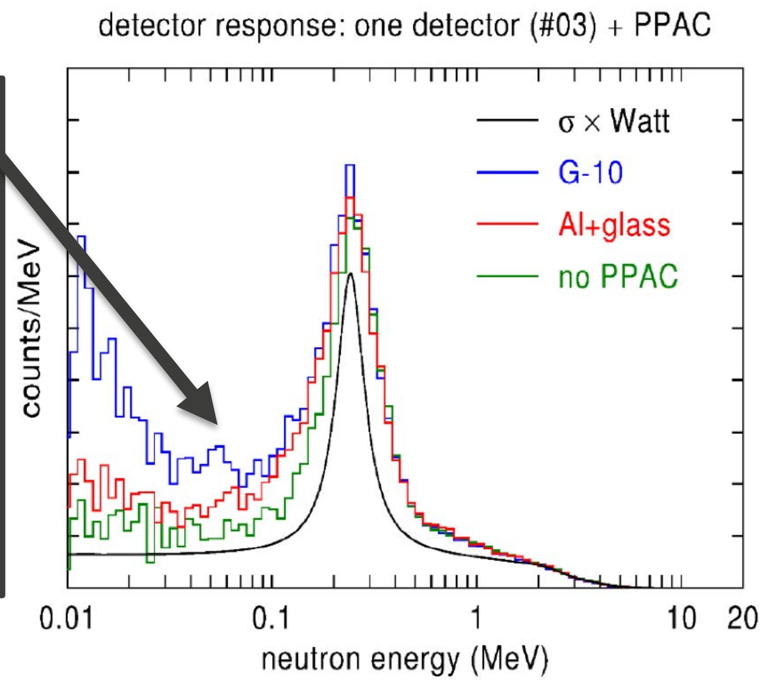
- **The Chi-Nu team, which includes the nuclear data evaluator, used the information gleaned from their experiments and additional MCNP analysis to assign new systematic errors to the historical data set**
  - In particular, few measurements fully accounted for neutron scattering
  - Other issues were found in background assessments, detector efficiency and resolution
  - Corrections might have been possible if enough documentation had been provided
  - Postulated corrections would, mostly, move data towards more consistency
- **The ASC nuclear physics project has put considerable effort into improvements to the nuclear theory tools used for these evaluations**
  - The evaluation tools now include multi-chance fission; i.e. neutron emission before fission
  - (n,Xn'f) neutrons from high incident energy neutrons include pre-equilibrium
  - These have significant influence on the mean energy above second chance fission
  - Finally, the evaluation tools now include individual components of the systematic error allowing for cross correlations between experiments to be handled more correctly

The spread of evaluated mean energies ranges between 50 and 200 keV with even larger discrepancies (10-100x) in the tails that drive radiochemistry reactions.



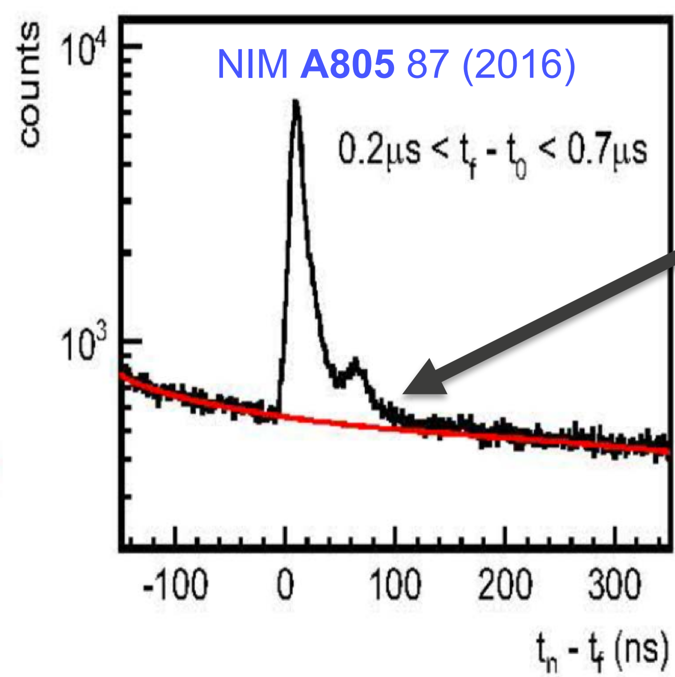
State of PFNS data
Circa 2006-2011





LLNL PPAC target was redesigned based on improved knowledge of scattering issues.

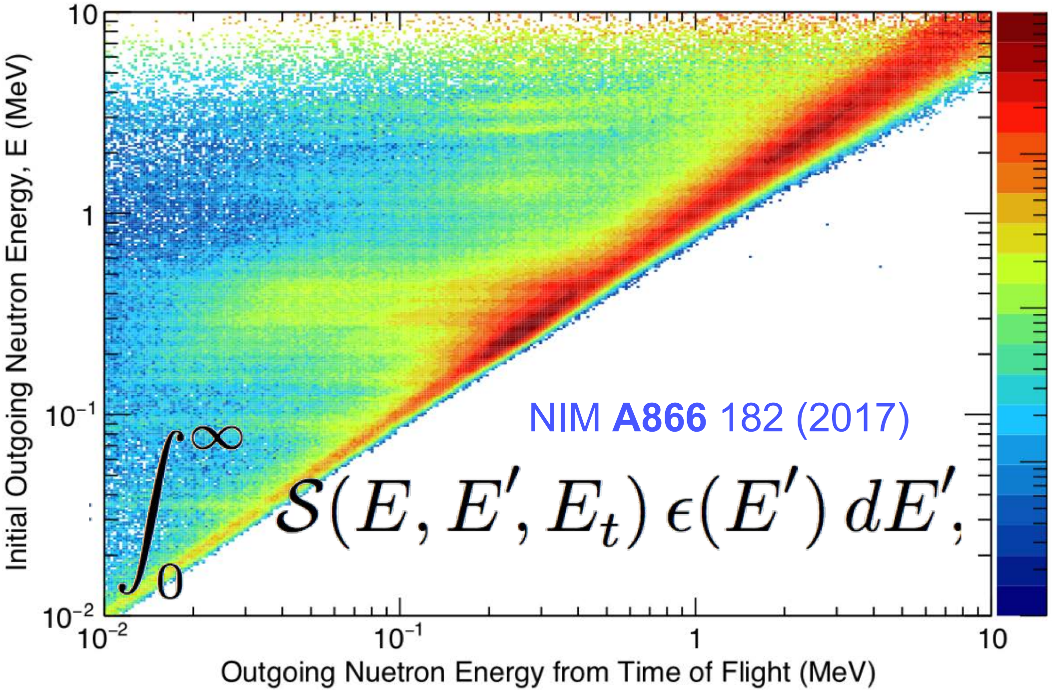
Staples, on which ENDF/B-VI and -VII are based, quoted scattering issues as "negligible" when in fact they are the dominant source of systematic bias.

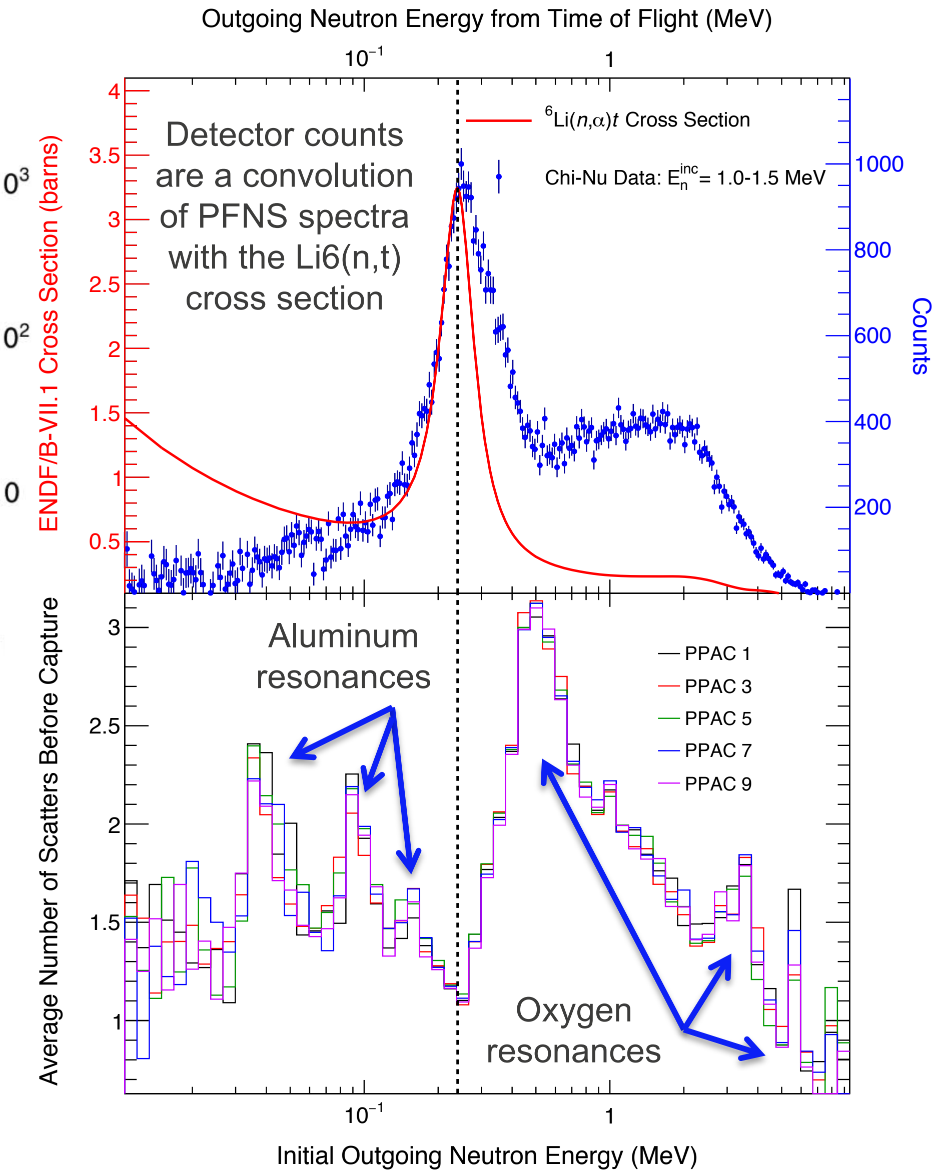


Modern DAQ systems can record (almost) the entire data stream and allow us to replay it afterwards. This allows for data analysis to be optimized after-the-fact, including accidental coincidence backgrounds.

See also NDS **123** 146 (2015)

MCNP analysis using HPC class resources has been essential for untangling multiple scattering…

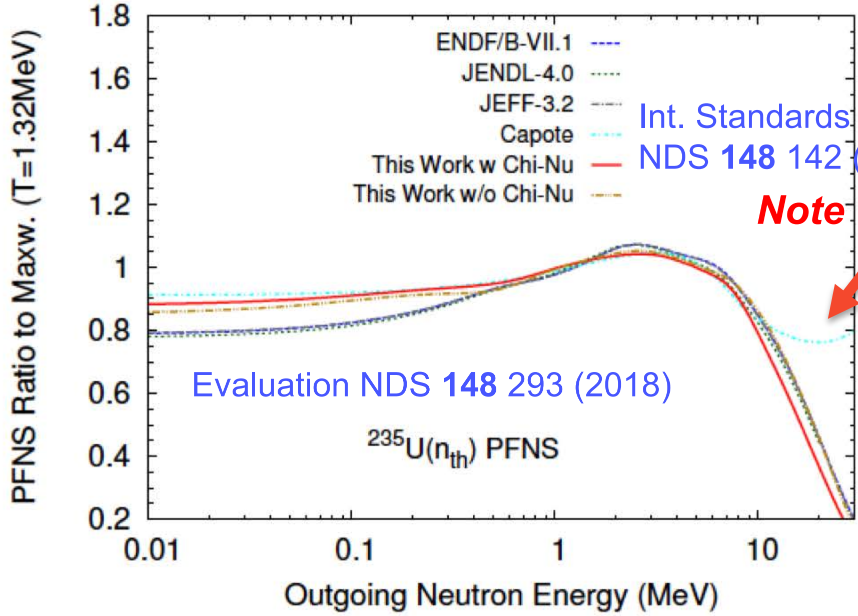




- Historical analysis uses the “known” flight path length and the measured delta-Time to directly infer the neutron energy
- *This is wrong* – the analysis must account for scattering that changes the actual flight path length

ENDF/B-VIII.0 Uranium-235 PFNS Evaluation

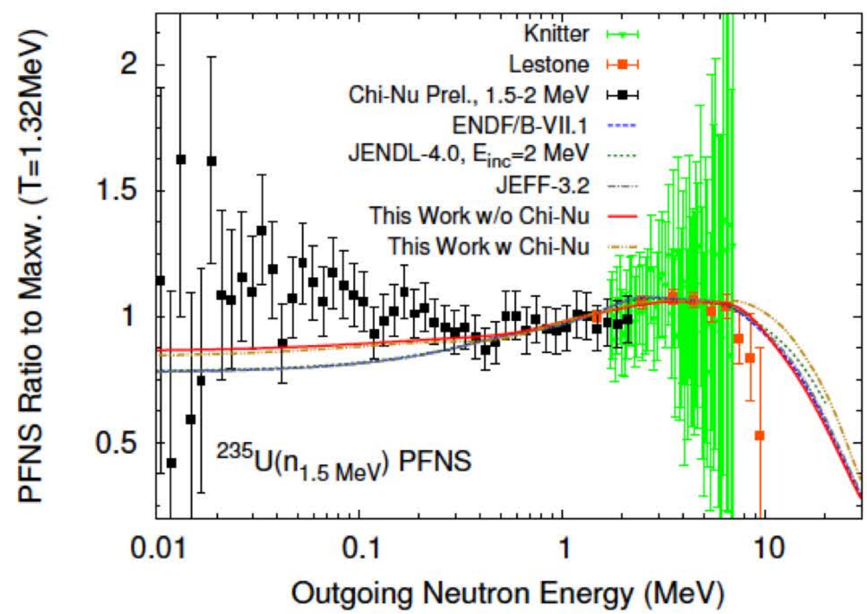
Much of this work under IAEA CRP (https://www-nds.iaea.org/pfns/)



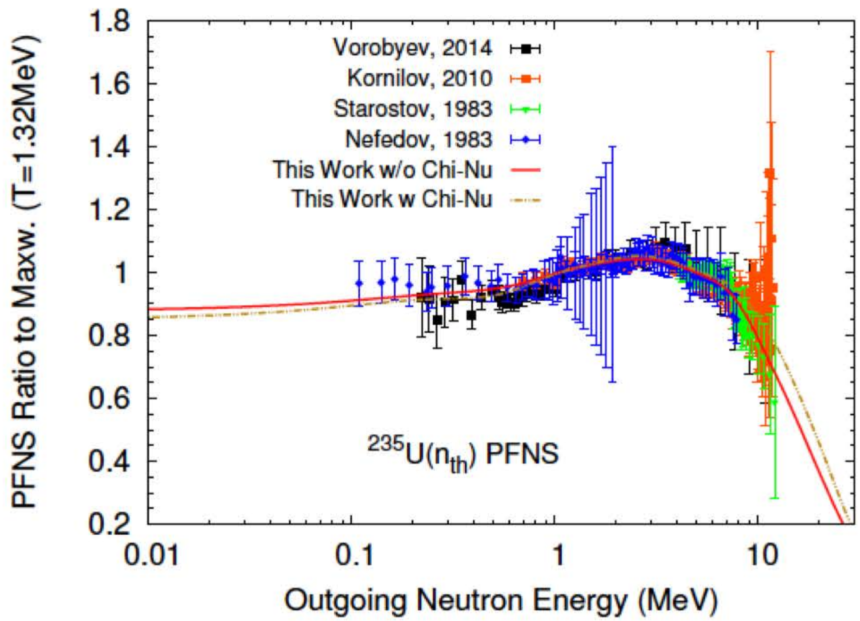
Int. Standards NDS **148** 142 (2018)

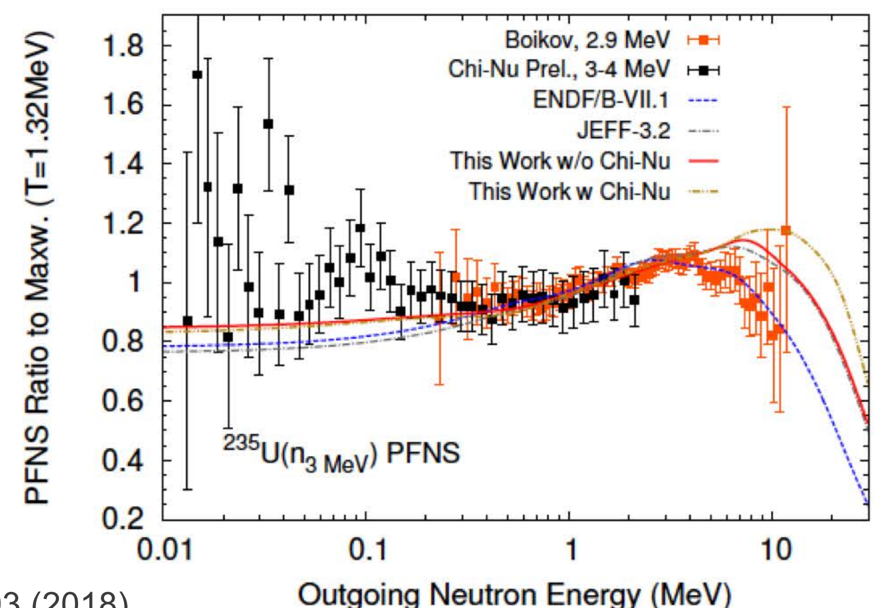
Note tail

Evaluation NDS **148** 293 (2018)



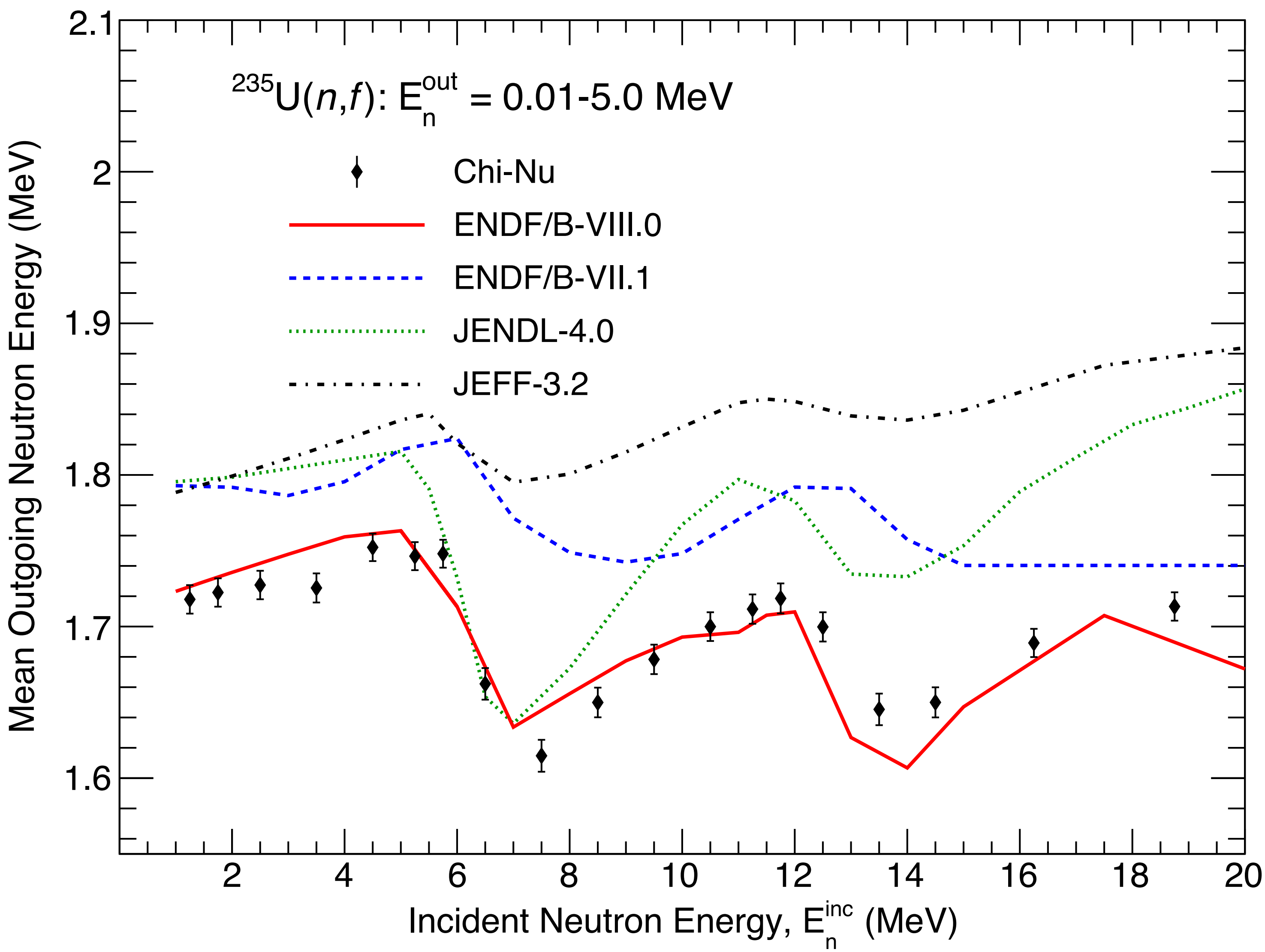
Chi-Nu data in black (LE) and red (HE) NDS **148** 322 (2018)





Figures from NDS **148** 293 (2018)

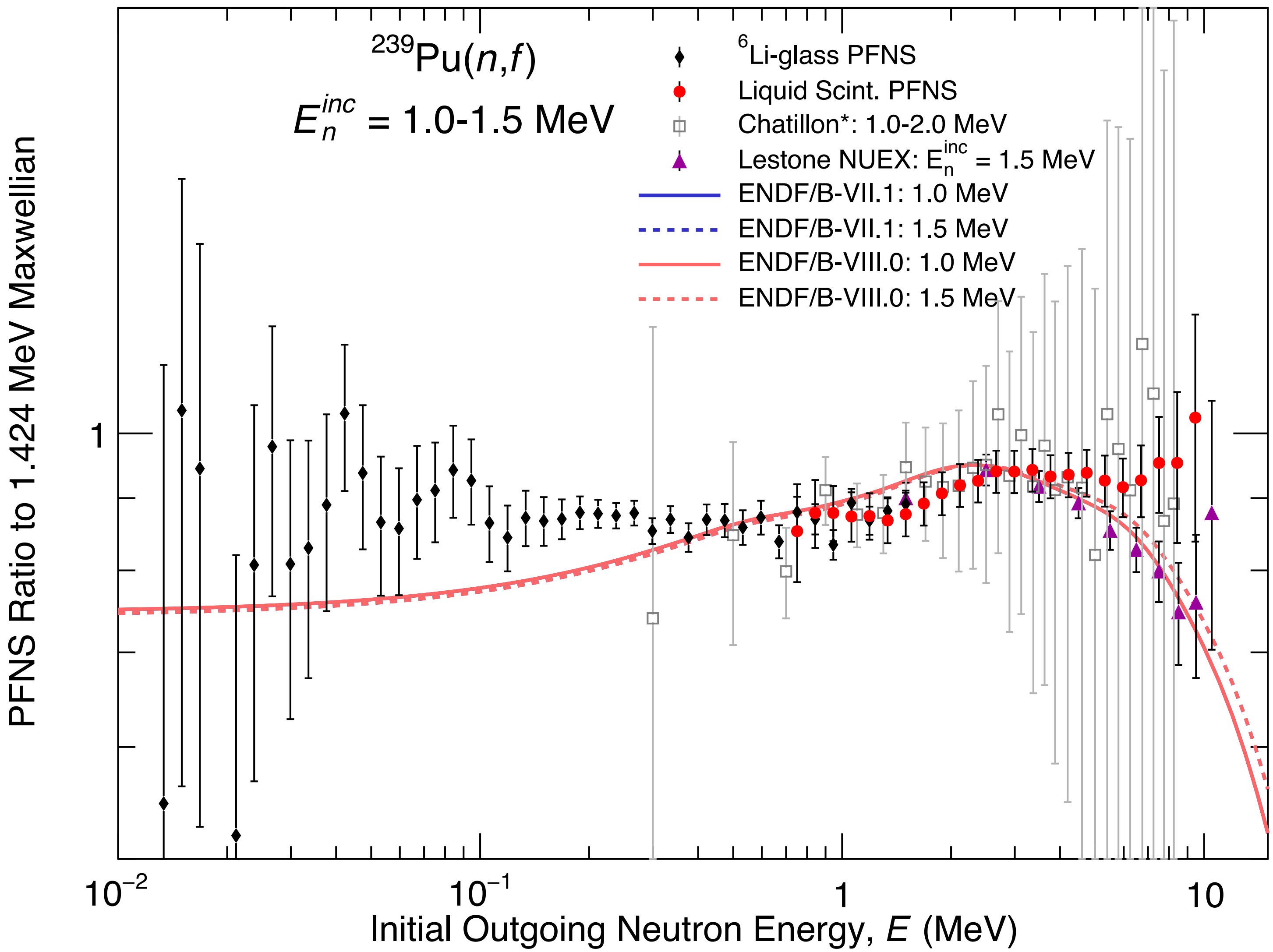
ENDF/B-VIII Uranium-235 average emission energy has been greatly reduced and <E> shape captured



Please note, the following Chi-Nu Pu239 PFNS data are *preliminary*.
Refinements in the mean values and uncertainties will change the final values.

ENDF/B-VIII adopted ENDF/B-VII PFNS up to 5 MeV
Preliminary Chi-Nu data indicate a slightly softer spectra

Plutonium-239 PFNS does not seem to soften as much as uranium-235



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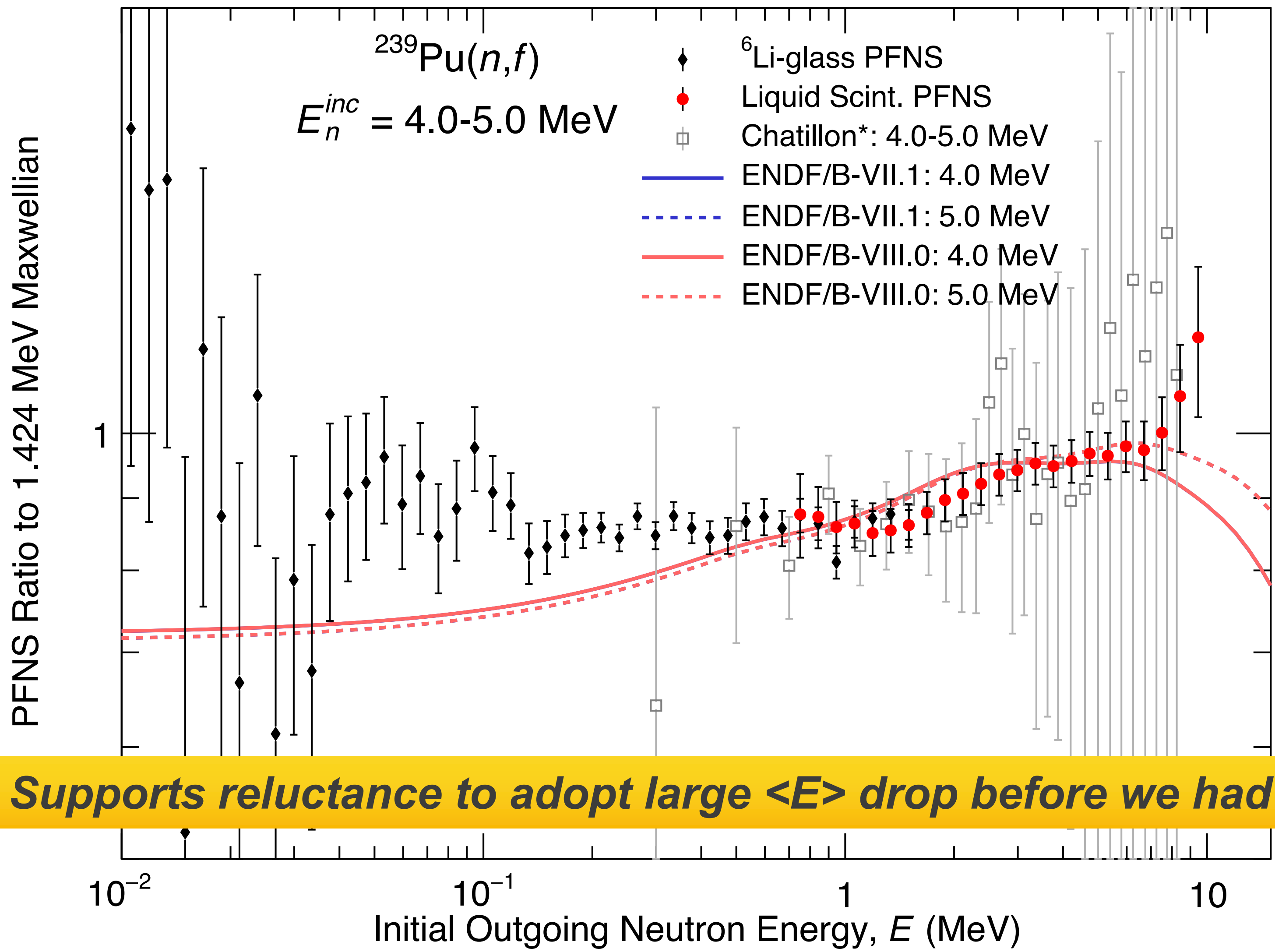
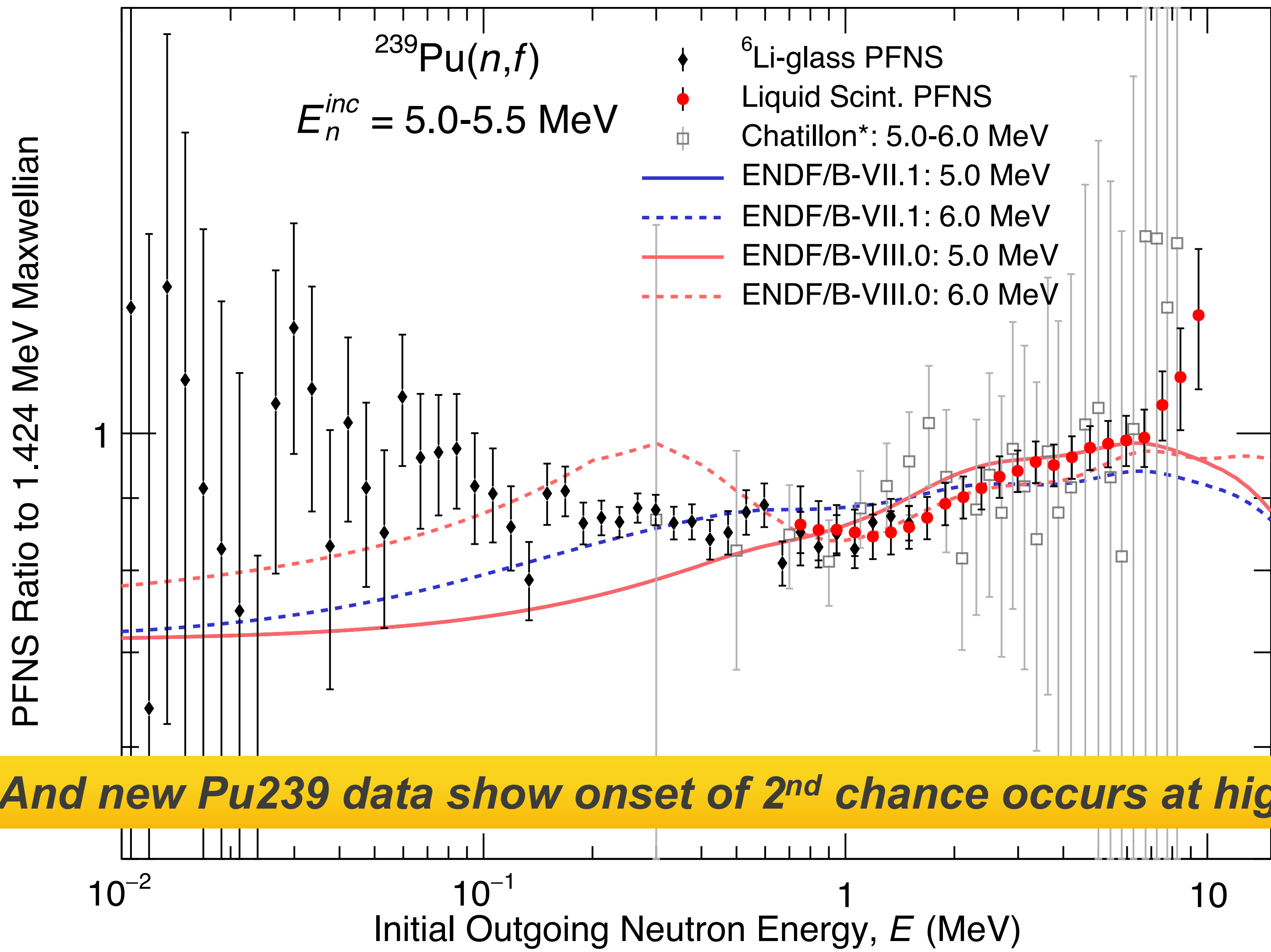


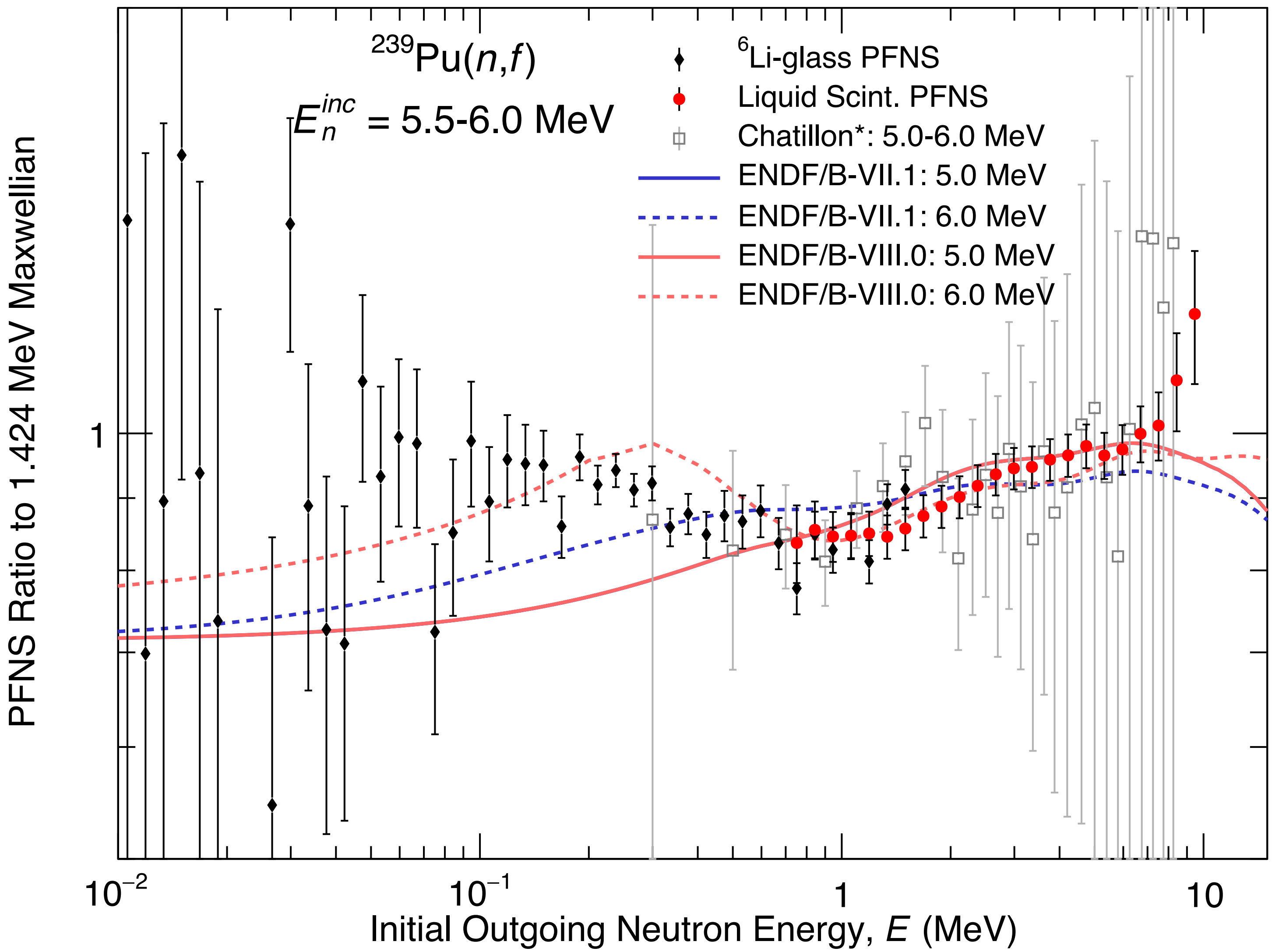
Supports reluctance to adopt large <E> drop before we had these data.

ENDF/B-VIII Plutonium-239 PFNS now includes better multi-chance fission physics that Chi-Nu confirms



And new Pu239 data show onset of 2nd chance occurs at higher energy.

ENDF/B-VIII Plutonium-239 PFNS now includes better multi-chance fission physics that Chi-Nu confirms



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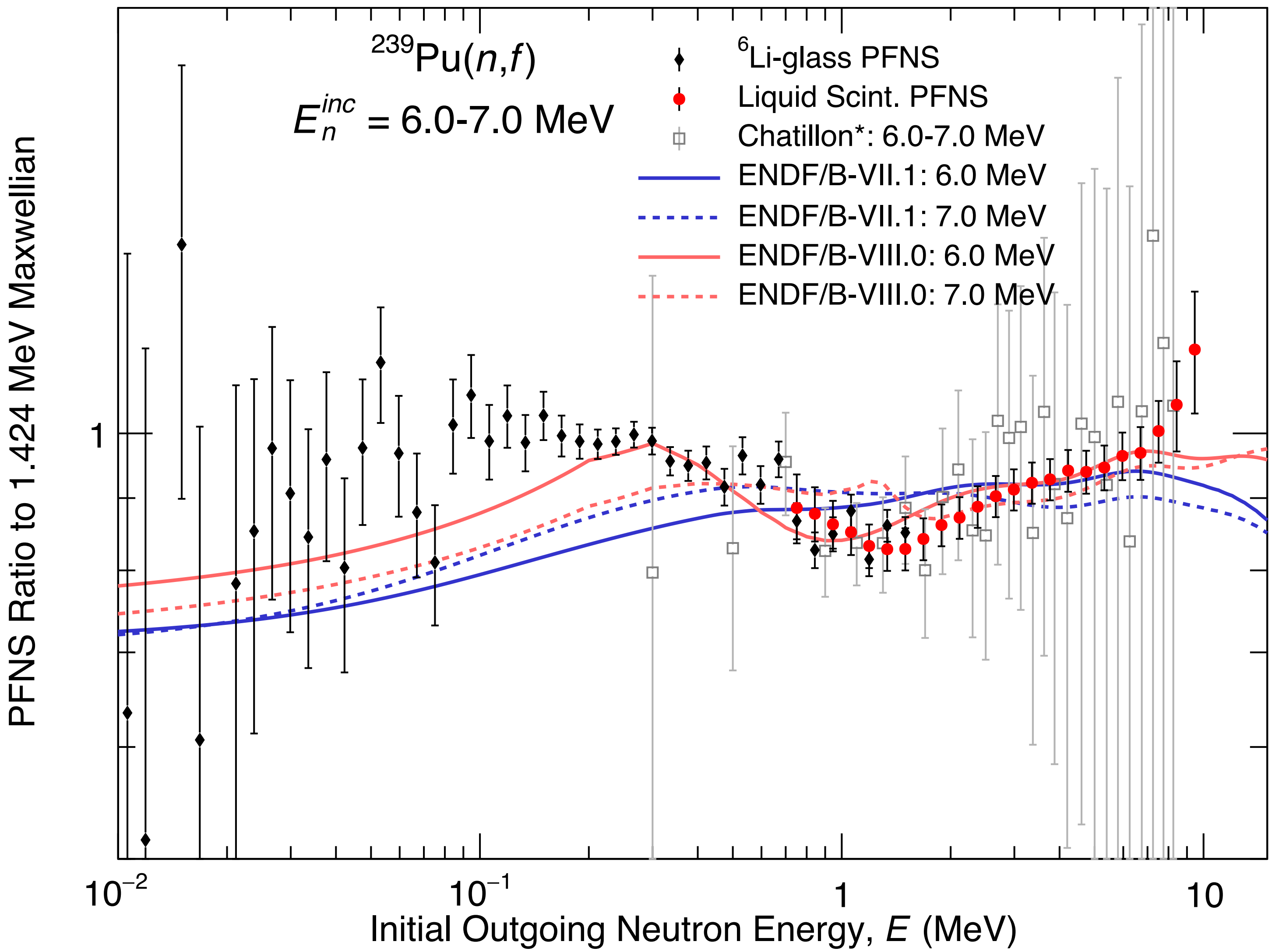
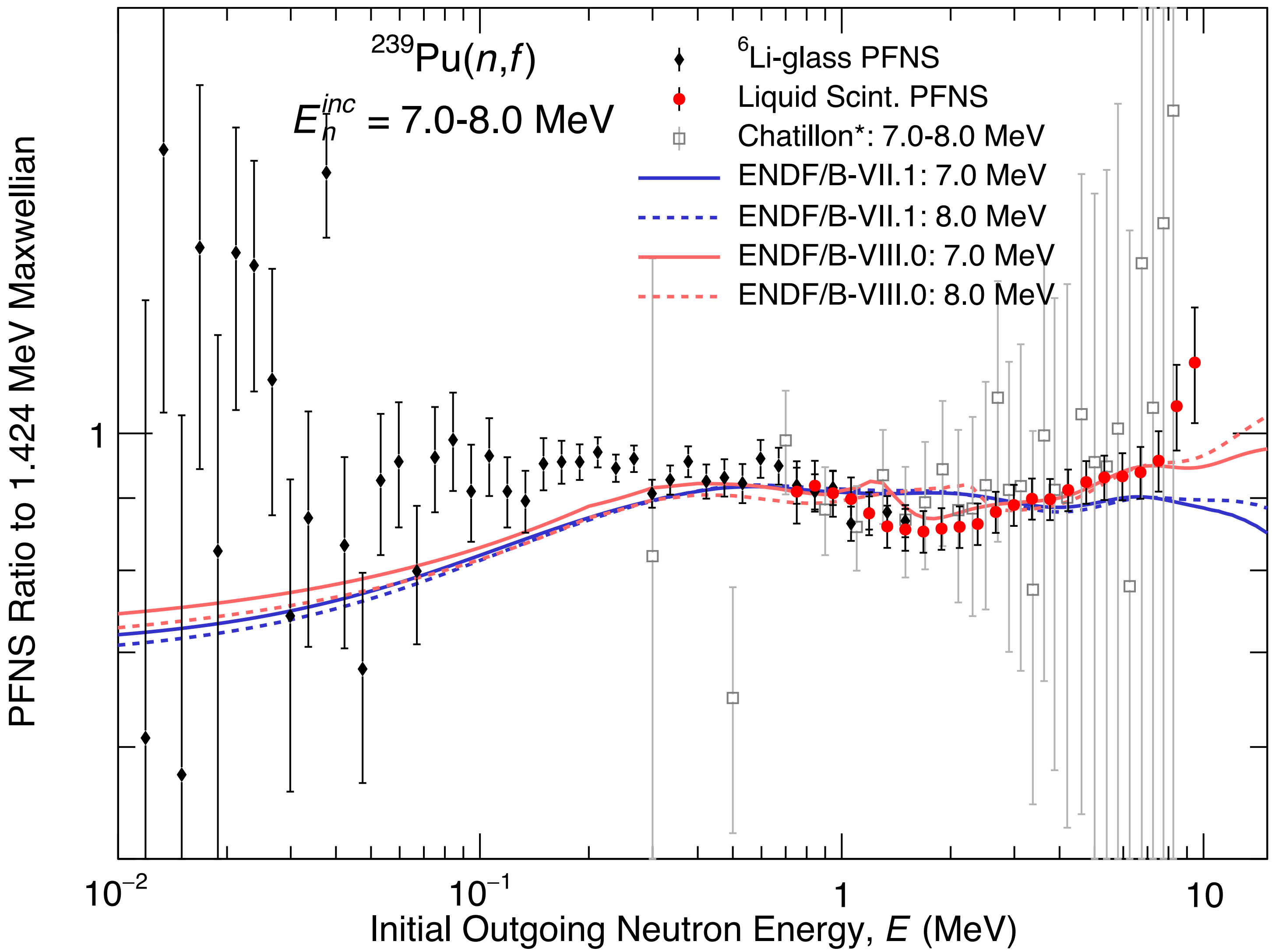
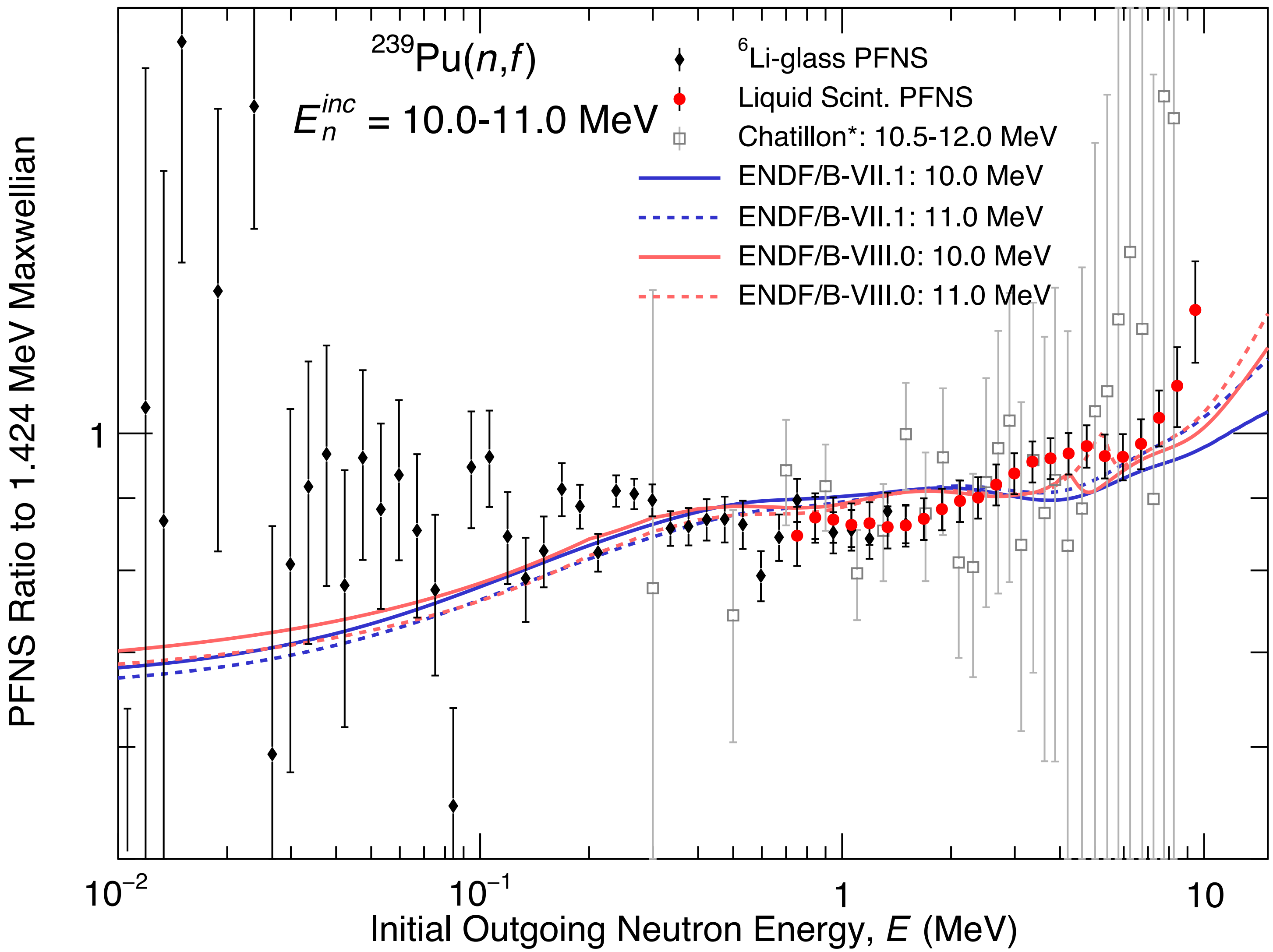


ENDF/B-VIII Plutonium-239 PFNS now includes better *and pre-equilibrium physics* that Chi-Nu confirms



ENDF/B-VIII Plutonium-239 PFNS now includes better *and pre-equilibrium physics* that Chi-Nu confirms



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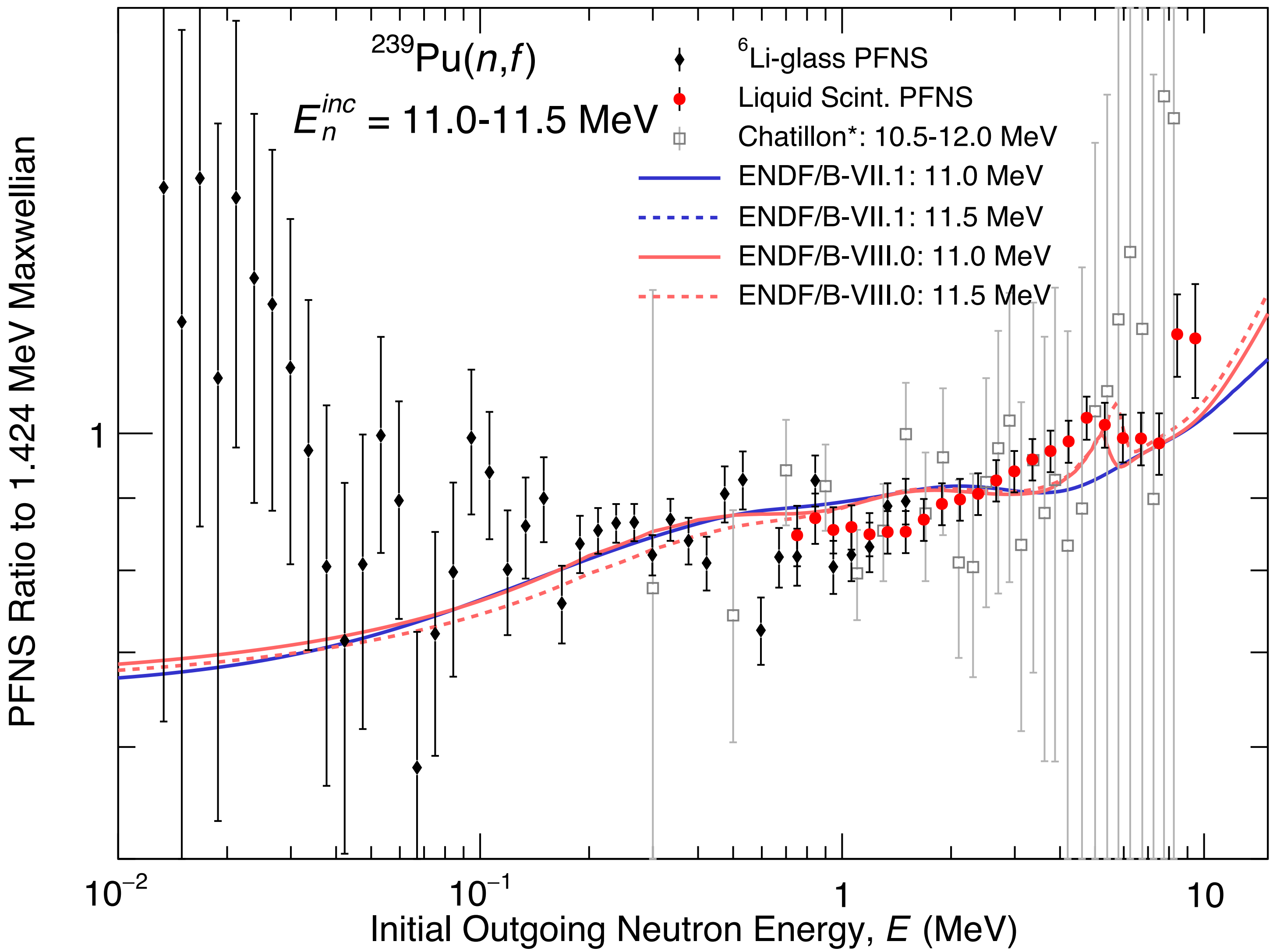

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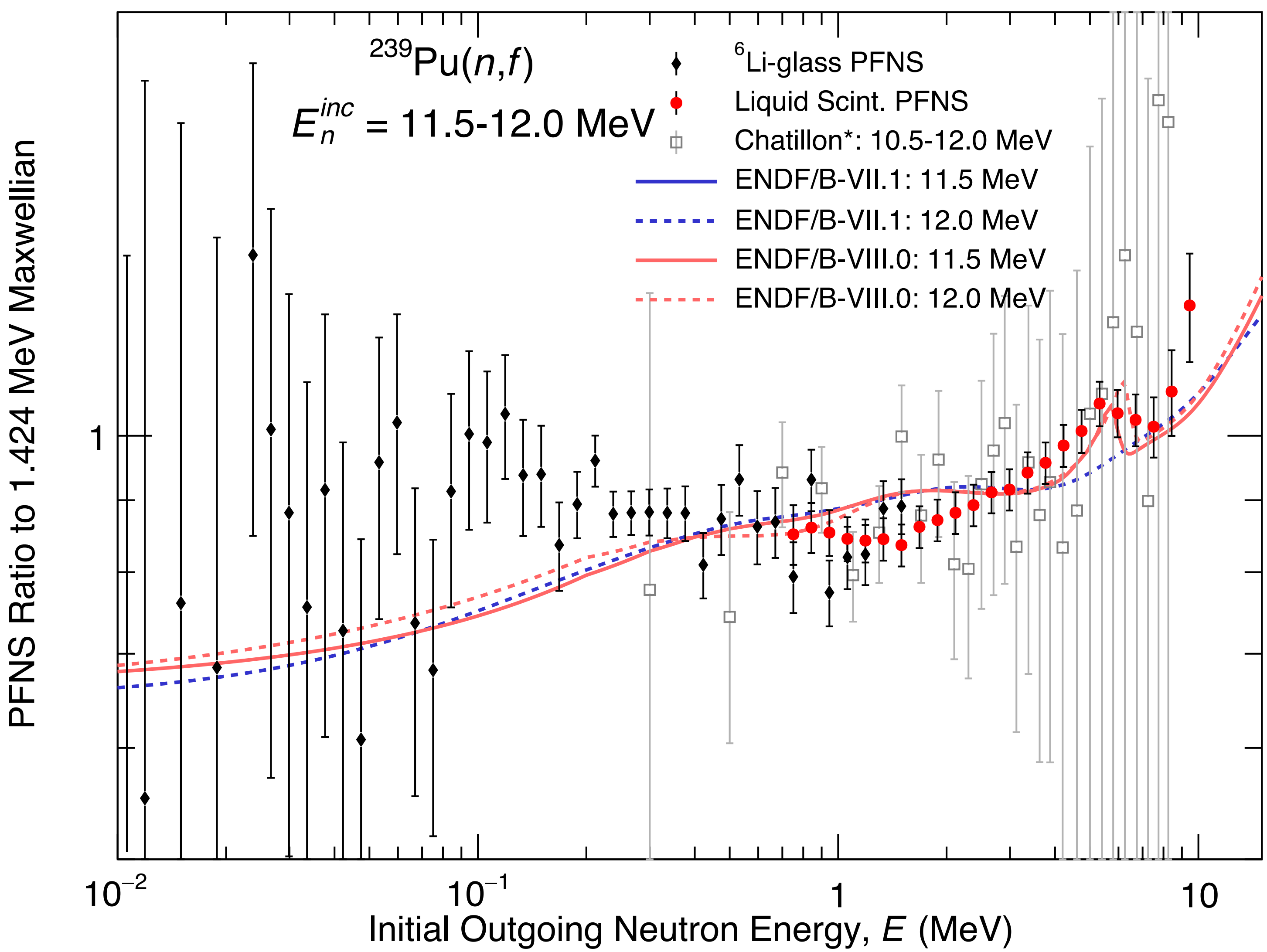

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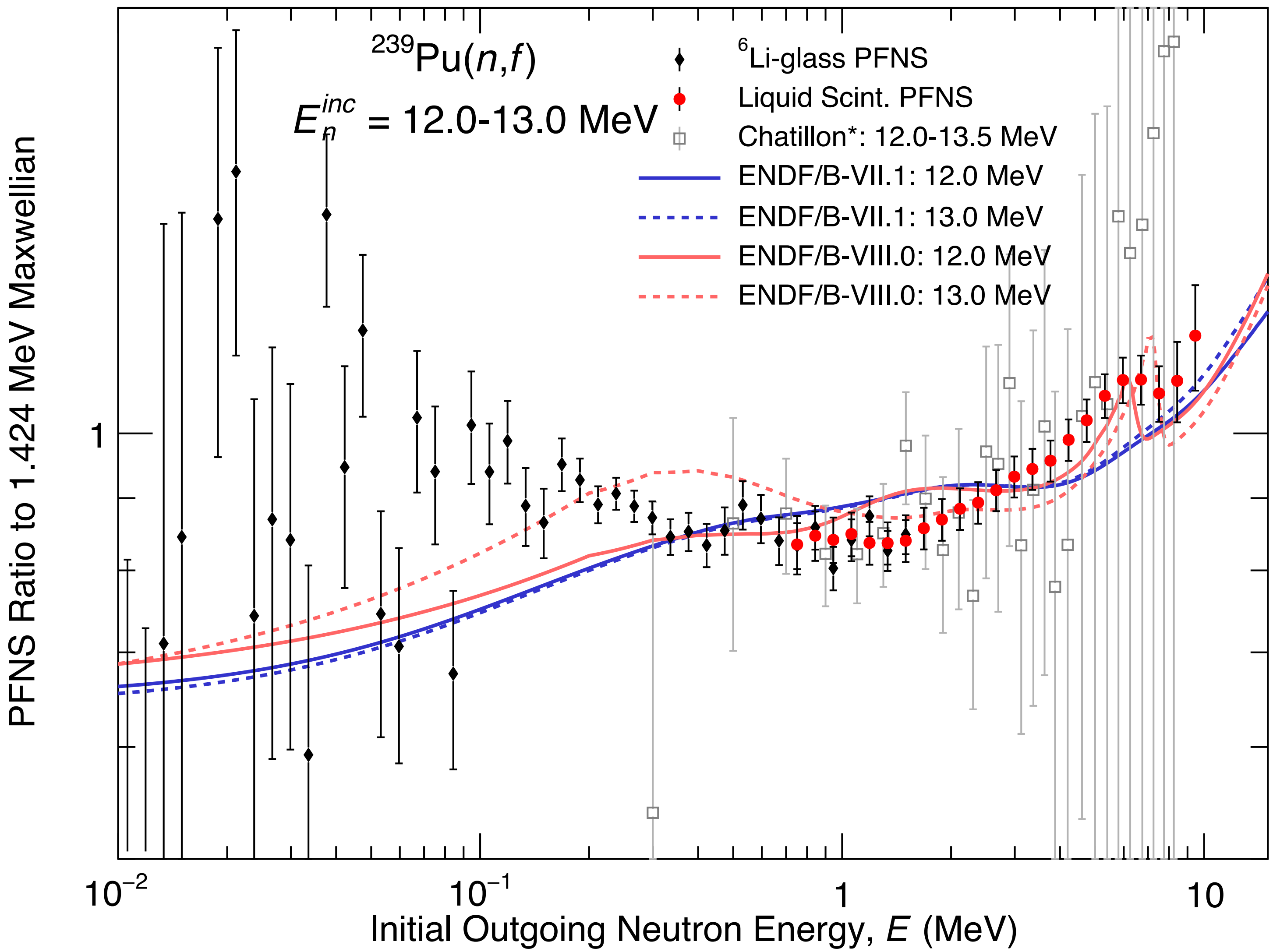

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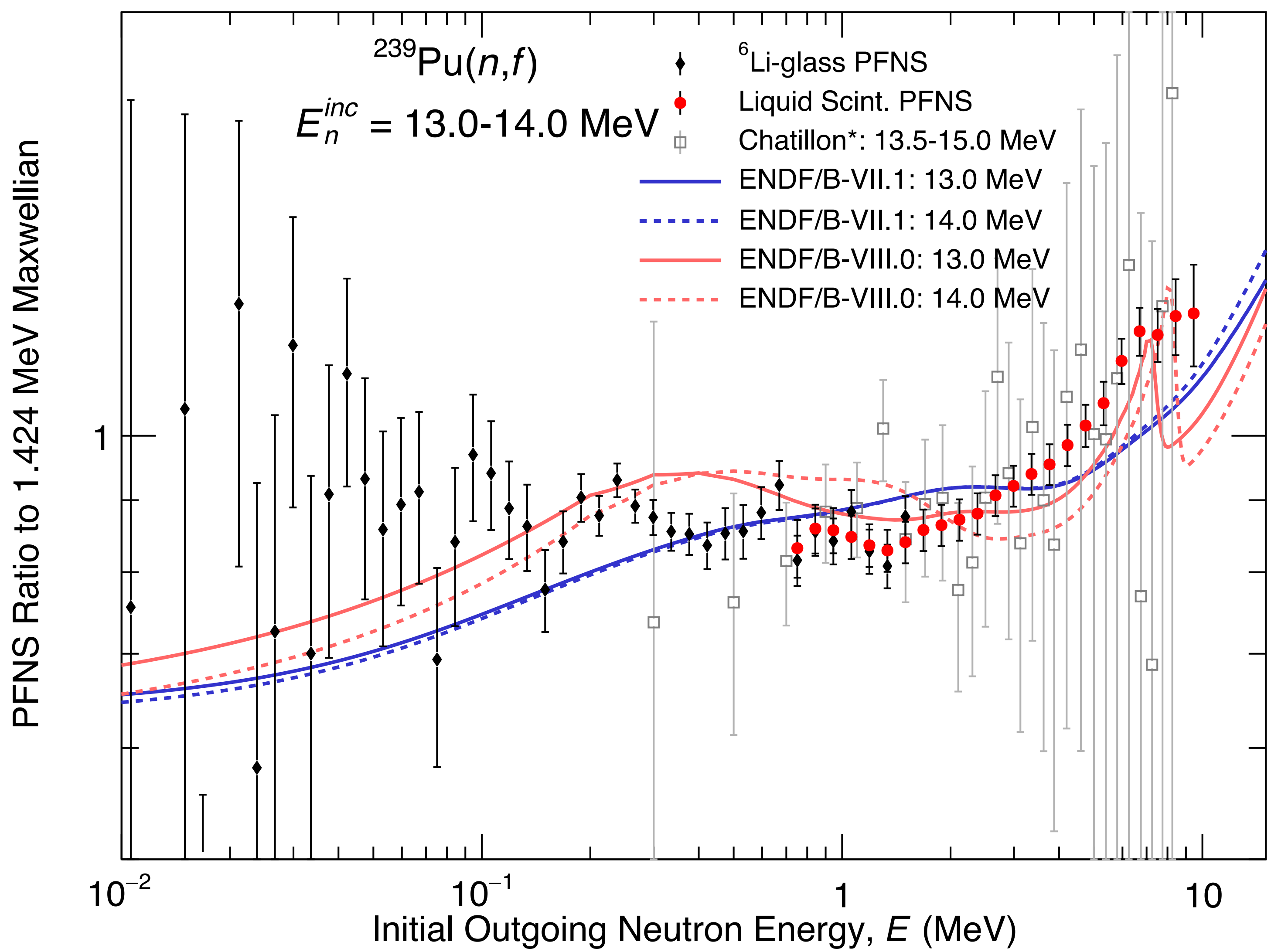

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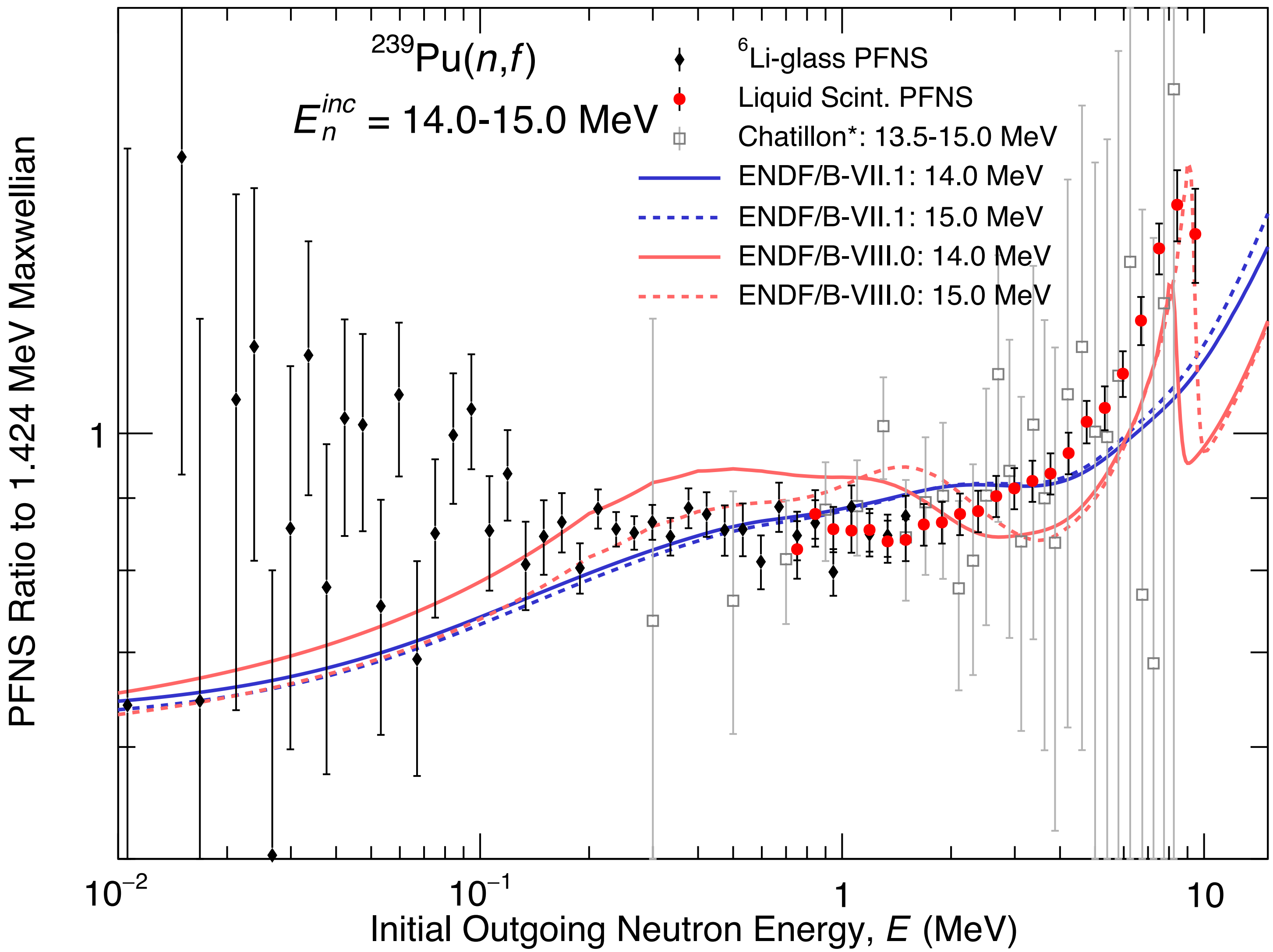
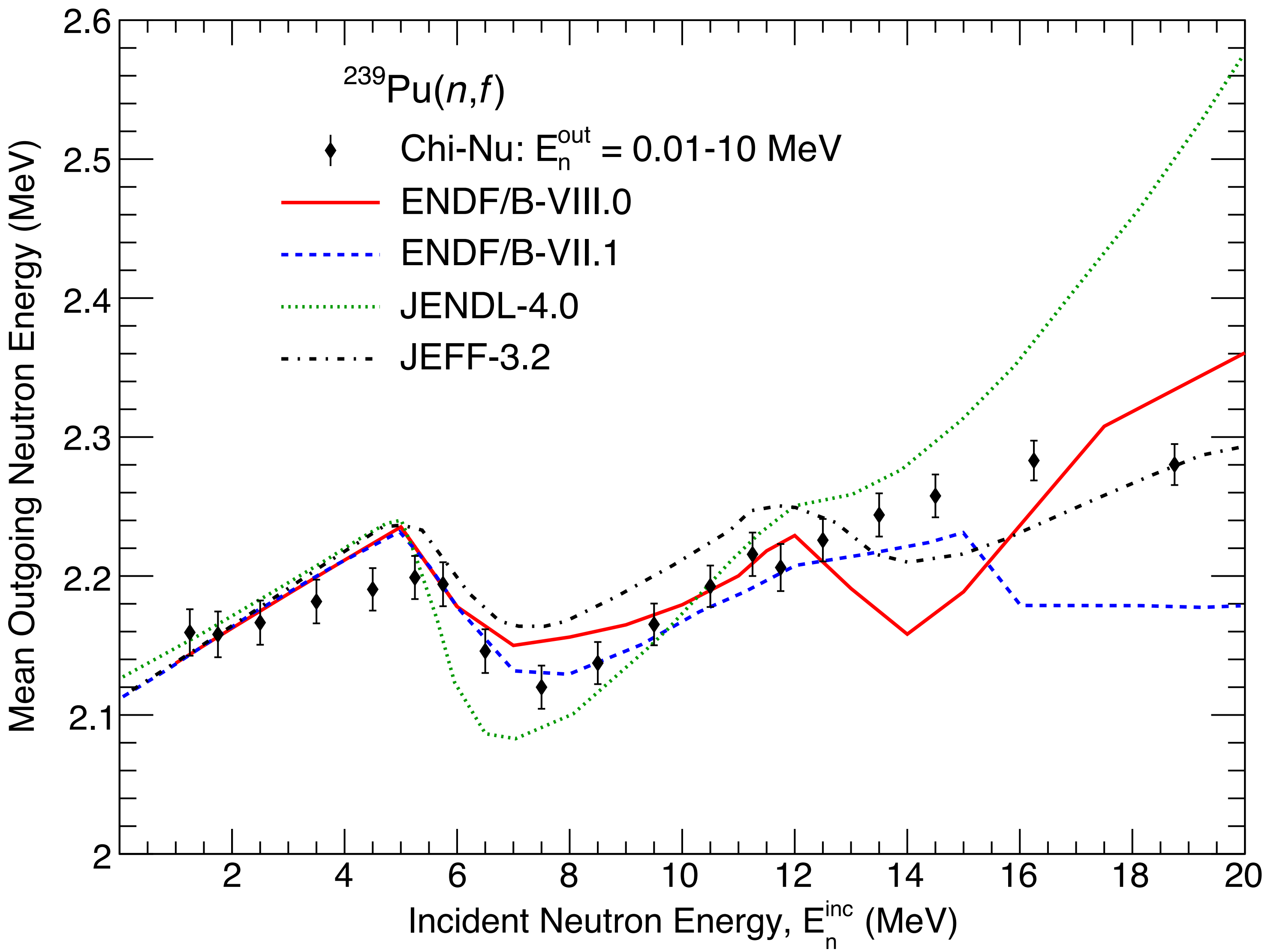


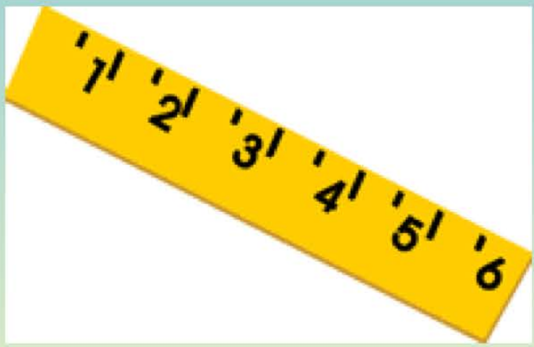
ENDF/B-VIII Plutonium-239 mean emission energies are still a bit high but accounted for in uncertainties



Pu239 Prompt Nubar (average # neutrons emitted)
The fission source term: $\Psi\ \nu\ \sigma\ \chi$

nubar

Unknown unknowns: estimating the unrecognized systematic uncertainty?



Ruler uncertainties:
Systematic unc. = 0.25

Independent of the number of measurements !!

Can we estimate the 0.25 if we do not know it?

E.V. Gai & S. Badikov (2003-2007)

Our measuring TOOL
TOF, fiss.chambers, …

Tool uncertainties:
Partially unknown syst. uncertainty

^{252}Cf(sf) nubar measurements unrecognized syst. uncertainty (USU) ?

111	Boldeman	1977		3.7549
116	Spencer	1982		3.7831
121	Hopkins	1963		3.7767
125	Asplund	1963		3.7910
127	White	1968	+1.5%	3.8194
128	Axton	1985A		3.7547
129	COLV/AXT	1966	-0.9%	3.7299
130	COLV/ULL	1965		3.7405
138	Alek-Rov	1981		3.7618
139	Smith	1984		3.7678
140	Edwards	1982		3.7641
141	Boz-nesh	1977		3.7475
142	DeVolpi	1972		3.7507
143	Zhang	1981		3.7534
144	Spiegel	1981		3.7828

All measurements:

3.765 +/-0.023 (0.6%)

If we drop outliers:

3.764 +/-0.016 **(0.4%)**

USU actin. nubar: 0.4%

GMA value (GLSQ):

3.764 +/-0.005 (0.13%)

Covariance Workshop CW2017
Aix-en-Provence, 2-6 October 2017

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There are two nubar measurement techniques
And they disagree by more than their stated error

An inspection of the mean values adopted by Hanna et al [1] for the different methods of measurement , as reproduced in Table 1, shows that the published experimental values can be grouped essentially into two sets of results, which differ by about 2% and which are strongly correlated with the methods of measurement. In fact, while the measurements performed with large liquid scintillators give values close to 3.80 neutrons per fission, the results depending on the boron pile and the manganese bath give for $\bar{\nu}_t$ an average value close to 3.70. This spread of values, of the order of three times the reported standard errors, exceeds those to be expected from a Gaussian distribution of statistical errors and cannot be explained by the remaining uncertainties in the

Page 7 of the International Nuclear Data Committee document INDC(NDS)-34/G, Status of the Energy Dependent nubar Values for the Heavy Isotopes (Z greater than or equal 90) from Thermal to 15 MeV, and of nubar Values for Spontaneous Fission. F. Manero, V.A. Konshin. Vienna, July, 1972.

And yet the standards of the time adopted the mid-point and gave it an unreasonably small uncertainty

It should be pointed out that, in spite of the apparent high accuracy of the value of $\bar{\nu}_t^{sp}(^{252}Cf)$ adopted as standard, its actual uncertainty may be considered as large as $\pm$ 1.2% (namely $\sigma_{\bar{\nu}}$ = 0.047), according to the spread in the experimental values. Such an uncertainty should be taken into consideration, therefore, in those measured $\bar{\nu}$ values in which $\bar{\nu}(^{252}Cf)$ was used as standard.

1969 ‘standard’ Californium-252 nubar 3.743 +/- 0.016 (0.4%)
Hanna et al., Atomic Energy Review, Volume VII, No. 4, 3 (1969)

In the early 1970s, they were trying to justify 0.4% instead of 1.2%.

How did we get to a belief that 0.13% was rational?

Page 10 of the International Nuclear Data Committee document INDC(NDS)-34/G, Status of the Energy Dependent nubar Values for the Heavy Isotopes (Z greater than or equal 90) from Thermal to 15 MeV, and of nubar Values for Spontaneous Fission. F. Manero, V.A. Konshin. Vienna, July, 1972.

A comprehensive reanalysis of every measurement was done multiple times, often by the experimentalist but with direct peer review …

7. Energy dependent measurements of $\bar{\nu}$ for ^{239}Pu

Mather et al. [140] used also the large liquid scintillator technique to measure average values of $\bar{\nu}_p$ of ^{239}Pu over 11 energy bands below 1.2 MeV. The energy bands were 40 - 115 keV, 115 - 285 keV and 100 keV wide intervals above 300 keV. In the interval 525 keV to 875 the measurements were re-peated with 50 keV wide energy bands. The relative accuracy in both series of measurements was ~1%.

Given some uncertainty on californium nubar, it must then be realized that all other nubar measurements are relative to this standard and must have larger uncertainties.

The spread in the data for plutonium-239 prompt nubar indicate approximately 1% uncertainty, at best…

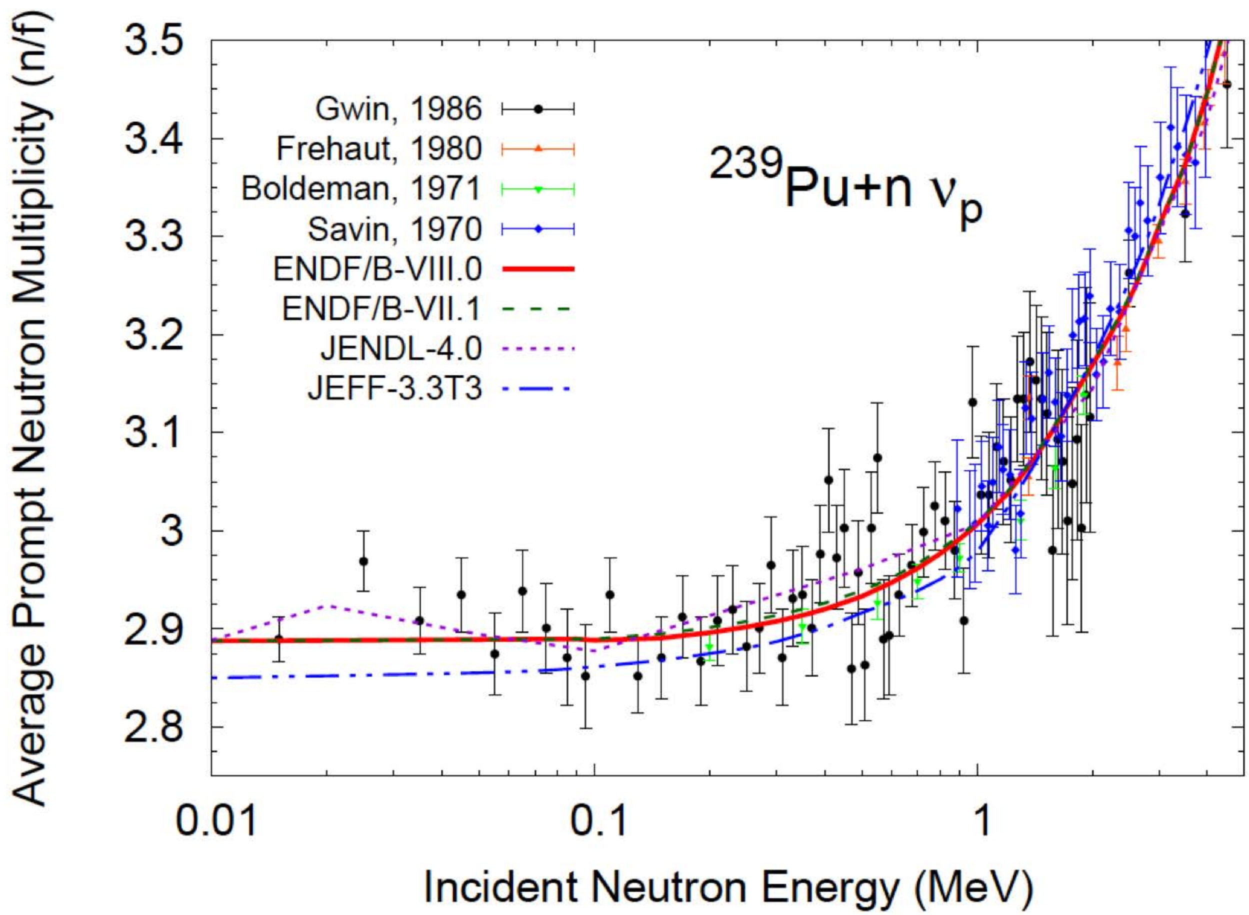


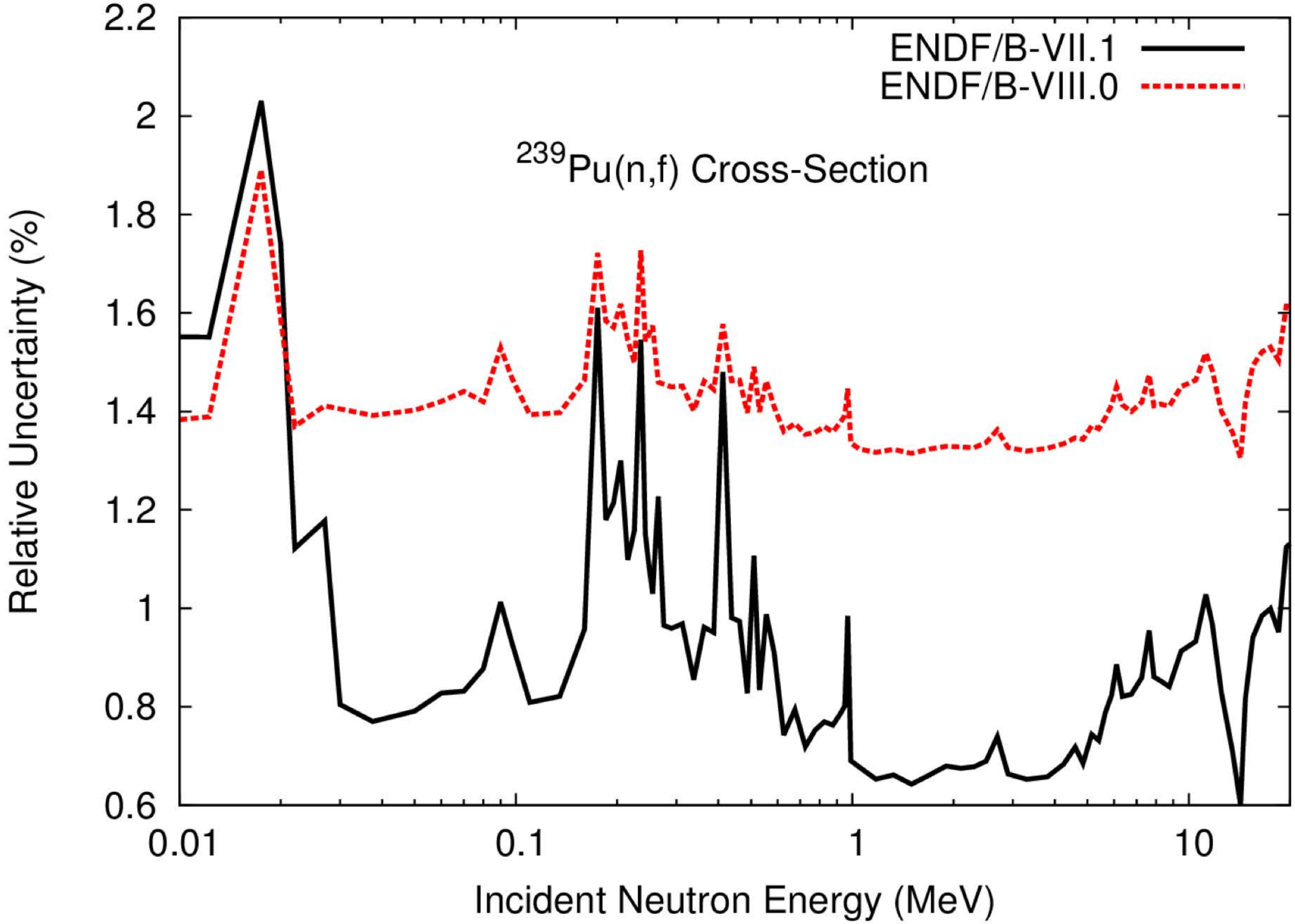
FIG. 77. (Color online) Evaluated ^{239}Pu(n,f) neutron induced fission prompt $\bar{\nu}_p$ in the fast region compared with data retrieved from EXFOR and with previous evaluations.

ENDF/B-VIII.0
NDS **148** 1 (2018)

Pu239 Fission Cross Section
The fission source term: $\Psi\ \nu\ \sigma\ \chi$

Fission xs

With similar justification to nubar, the fission cross section ruler was determined to have a 1.2% lower bound



Similar to nubar reviews, LANL (D. Neudecker) has undertaken a comprehensive review of fission XS

Unc. Source	Typical range	Correlations	Cor(Exp_1,Exp_2)
Sample Mass	> 1%	Full	Possible (same sample)
Counting Statistics	Sample-dependent	Diagonal	0
Attenuation	0.02-2%	Gaussian	Likely
Detector Efficiency	0-0.3%, 1-2%	Full < 10 MeV	Likely, 0.5-1.0
FF Angular Distrib.	~0.1%	Gaussian	Likely, 0.75-1.0
Background	0.2 - >10%	Gaussian	Possible
Energy Unc.	1%, 1-2 ns	Arises from conv.	Technique-dependent
Neutron Flux	0%, >1%	Full-0.5	Technique-dependent
Multiple Scattering	0.2-1%	Gaussian	0.5-0.75
Impurit. in Sample	Sample-dependent	1.0-0.9	0.5-0.75
Dead Time	>0.1%	Full	0

A ‘template’ of expected uncertainty sources has been developed (LA-UR-17-29963) and a review of the experimental data base has begun.

Checking the database, it is clear many errors were not appropriately documented

Data Set	Data Type	Min δ	Max δ	Min E	Max E	EXFOR #
611	absolute	1.0	1.0	1.45E+01	1.45E+01	
644	absolute	2.0	2.0	1.45E+01	1.45E+01	30634
615	absolute	2.1	2.1	5.00E+00	5.00E+00	
1038	absolute	2.3	7.7	1.00E+00	5.50E+00	30670
640	absolute	2.4	3.1	1.50E-01	9.60E-01	10314
620	absolute	2.8	6.6	3.00E-02	9.80E-01	20567
⋮						
8002	ratio absolute ^{235}U(n,f)	0.7	3.8	2.00E-01	1.30E+01	14271
602	ratio absolute ^{235}U(n,f)	0.8	6.8	2.53E-08	1.00E+01	
654	ratio absolute ^{235}U(n,f)	1.0	5.7	2.40E-02	7.50E+00	
685	ratio absolute ^{235}U(n,f)	1.1	1.1	1.45E+01	1.45E+01	
653	ratio absolute ^{235}U(n,f)	1.2	6.9	1.20E-01	7.00E+00	40824
1014	ratio absolute ^{235}U(n,f)	1.3	1.6	8.50E-01	6.00E+01	13801
600	ratio absolute ^{235}U(n,f)	1.7	27.4	8.50E-04	3.00E+01	10562
605	ratio absolute ^{235}U(n,f)	1.7	15.3	5.50E-03	1.00E+00	20363
608	ratio absolute ^{235}U(n,f)	2.0	12.6	4.50E-02	5.00E-01	21463
609	ratio absolute ^{235}U(n,f)	2.0	2.1	1.00E+00	1.40E+01	21195
631	ratio absolute ^{235}U(n,f)	2.1	2.1	2.53E-08	1.50E-01	
1012	ratio absolute ^{235}U(n,f)	2.1	5.8	5.70E-01	2.00E+02	41455
⋮						
630	ratio shape ^{10}B(n,α)	2.3	5.0	2.53E-08	1.50E-01	

UNCLASSIFIED

Target Mass Intercomparison

NUCLEAR DATA AND MEASUREMENTS SERIES

ANL/NDM-48

^{235}U FISSION MASS AND COUNTING COMPARISON
AND STANDARDIZATION

by

W. P. Poenitz, J. W. Meadows and R. J. Armani

May 1979

- The 1970s were a heyday of high-precision experimental efforts
- Target fabrication and characterization capabilities were at their best ever
  - However, even then there are not enough samples to constitute a statistical sampling
- *So how do we handle lab-to-lab systematic errors in mass?*

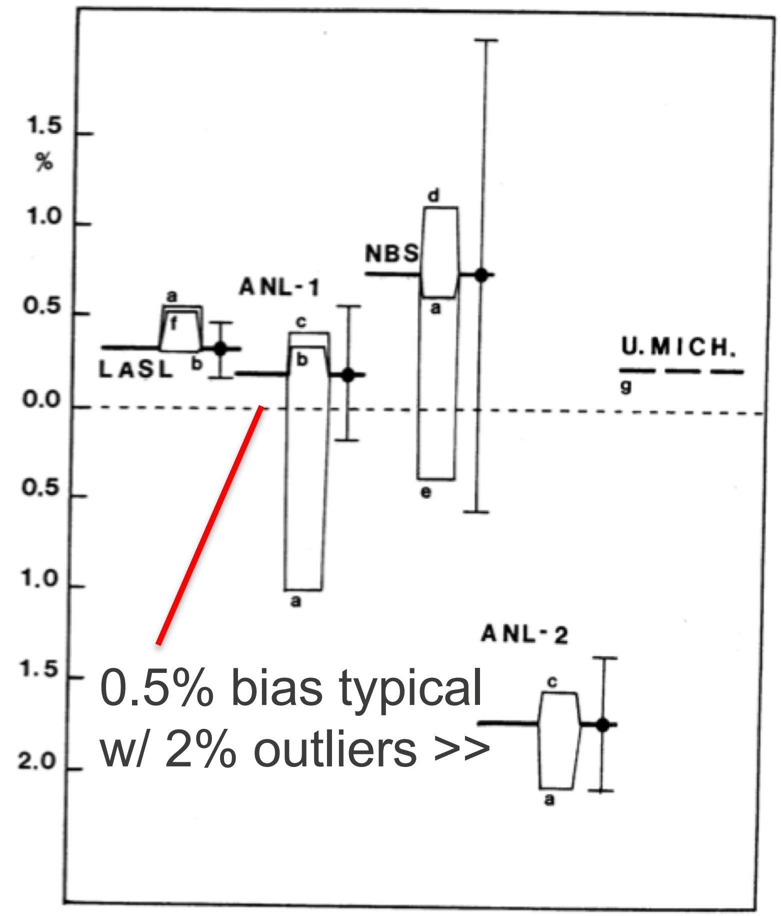


Fig. 3. Comparison of the Four Different Mass Scales Involed in the Present Intercomparison. Values are shown relative to a "unified mass scale" derived as an unweighted average. a = isotopic composition and half-life, b = isotopic dilution, c = colorimetric comparison with standard, d = thermal neutron comparison with quantitative deposition, e = thermal neutron comparison with ^{239}Pu sample, g = weighting.

Back to gates

Uncertainties in our fundamental data would have even larger impact without integral constraints.

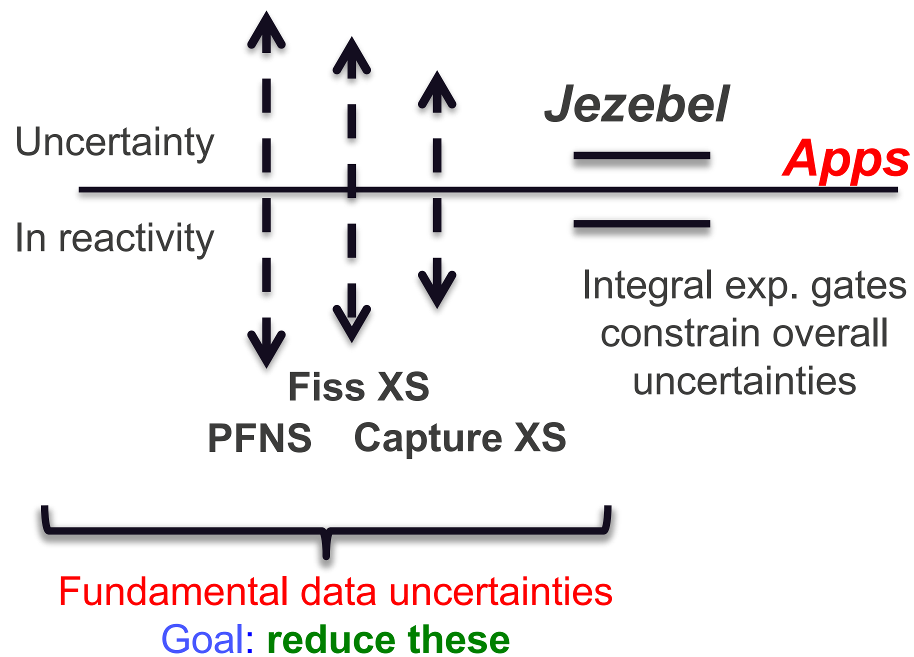
- Overall nuclear reactivity is constrained by exceptionally precise criticality experiments – especially Jezebel (bare Pu), Godiva (bare HEU), and SNM + reflectors (e.g. U, Be, Fe, Poly, …)
- But there are compensating errors in the XS components that drive reactivity that are much larger than this constraint.

- **One can get criticality right for the wrong reasons, and then get other things wrong, e.g. diagnostics, outputs and performance!**

- *-> example: a recent trial (softer) prompt fission neutron spectrum (PFNS) for Pu239 reduced the (n,2n) reaction rate in Jezebel by ~10% [Kahler LA-UR-14-28703] with implications on metrics like deltaP*

We rarely understand the impact of errors in isolation.

They interact, often in unexpected ways.



A high-quality bare plutonium critical assembly is essential first gate for plutonium-239 neutron reactivity.

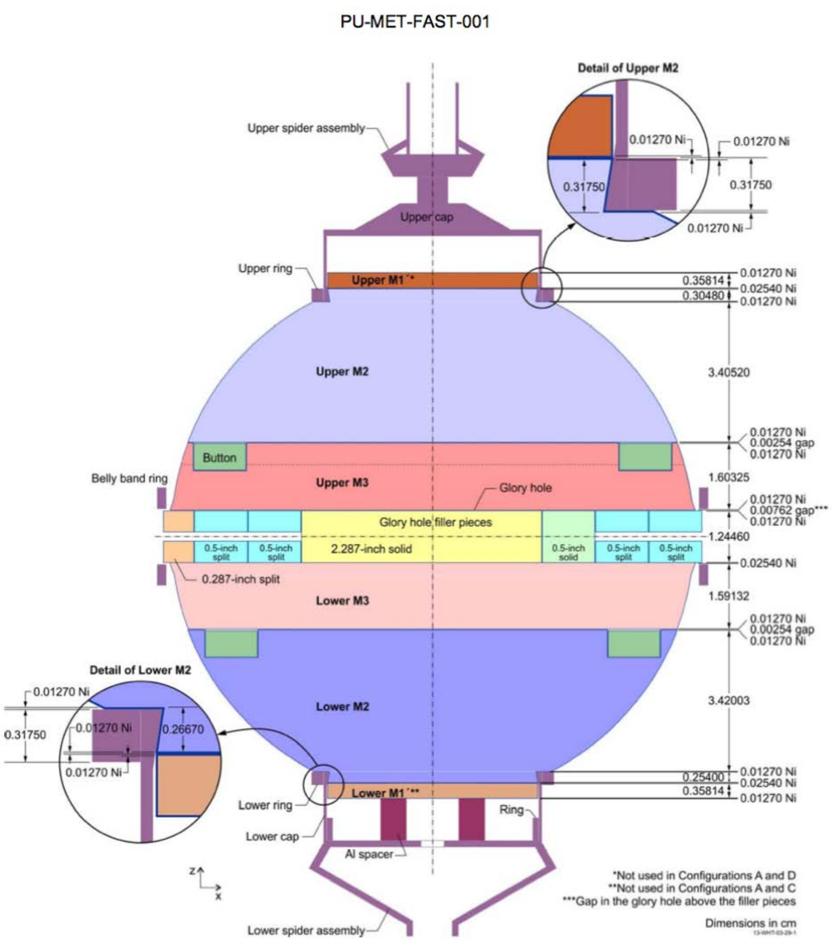


Figure 29. Assembly of Parts; View Plane Parallel to Glory Hole.
(Dimensions are in centimeters.)

Jeff Favorite at Los Alamos spent ~4 years digging through the archives in order to provide a complete re-assessment of the Jezebel critical assembly. This resulted in an updated specification PU-MET-FAST-001 rev. 4 published September 30, 2016.

Unfortunately, the final specification miss-reported the total error. The density uncertainty dominates the total error budget. There are four 4 kg parts whose density uncertainty is fully correlated; when accounting for this the quoted uncertainty should be 0.00234 instead of the 0.00110 value quoted in the specification. [ref XCP-3:16–038(U)]

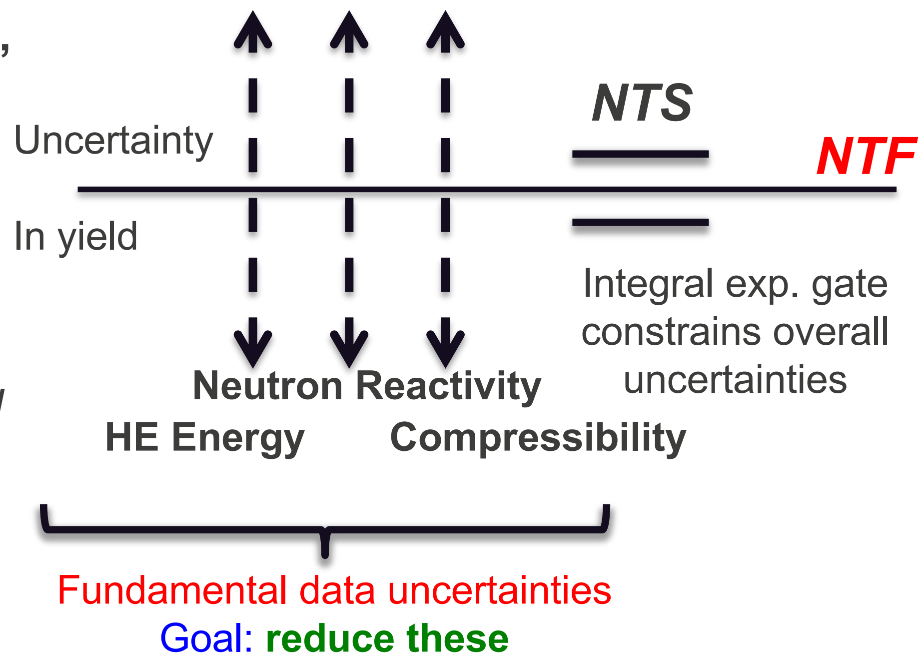
Despite his heroic efforts, the final mean value rests on a pencil notation of the density from notes on the wrong drawing.

The use of gates to tune compensating errors has broader implications…

- Overall the yield of an implosion system is constrained by our nuclear test history.
- But there are compensating errors in the physics that govern our predictive capability that are much larger than these constraints.

There is nothing new about adjusting fundamental data to get a 'known' answer. We have been doing this forever.

- **One can get yield right for the wrong reasons, and then get other things wrong, e.g. diagnostics, outputs and performance!**
- *Are there cliffs hidden in other solutions?*
- *How can we inform the physics using the integral constraints? How do we do this fairly?*



Some last thoughts

Summary

- **We have systematically underestimated the true uncertainty in our data**
  - Often this has been through the failure to provide complete documentation, or the failure or inability to fully characterize important sources of uncertainty
  - We have begun comprehensive efforts to identify these issues and tackled many of the most important, but *there is considerable work still to be done* (e.g. elastic/inelastic)
  - The ‘covariance’ data, uncertainty estimates, associated with the ENDF/B-VIII.0 plutonium-239 evaluation have begun to incorporate many of these new assessments

- **This work highlights the issue of compensating errors**
  - We have lots of ways to get the right answer, so long as we know what it is

- **Given the importance of a bare critical assembly as the first gate for neutron reactivity, the open questions regarding Jezebel must be resolved**
  - This likely means cutting new metal and producing a high-quality new measurement